L13 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:393069 CAPLUS
DOCUMENT NUMBER: 131:43666
TITLE: Method for selective esterification of polyols
INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu; Bornscheuer, Uwe; Schmid, Rolf D.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

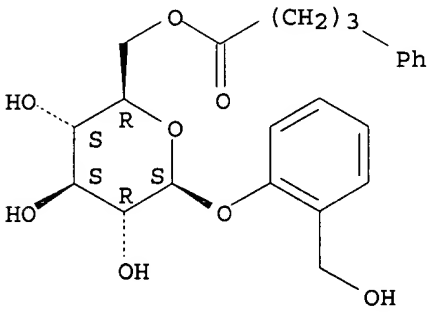
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

PRIORITY APPLN. INFO.: DE 1997-19753789 19971204
OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666

AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an esterase. The products have emulsifying activity with potential pharmaceutical use.

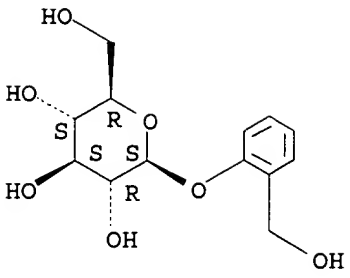
IT **218966-96-2P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(selective esterification of polyols)
RN 218966-96-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **138-52-3**, Salicin
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(selective esterification of polyols)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.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L13 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:393069 CAPLUS
DOCUMENT NUMBER: 131:43666
TITLE: Method for selective esterification of polyols
INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu; Bornscheuer, Uwe; Schmid, Rolf D.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

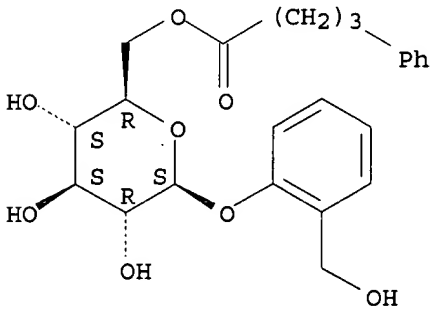
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

PRIORITY APPLN. INFO.: DE 1997-19753789 19971204
OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666

AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an esterase. The products have emulsifying activity with potential pharmaceutical use.

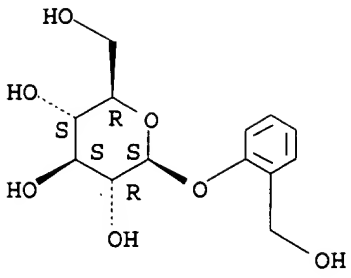
IT **218966-96-2P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(selective esterification of polyols)
RN 218966-96-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **138-52-3**, Salicin
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(selective esterification of polyols)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.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L13 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:83975 CAPLUS
DOCUMENT NUMBER: 136:123417
TITLE: Cosmetic and dermatologic compositions containing quercetin, rutin, salicin, and escin
INVENTOR(S): Hoffmann, Holger Walter
PATENT ASSIGNEE(S): Fribad Cosmetics G.m.b.H., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10034328	A1	20020131	DE 2000-10034328	20000714

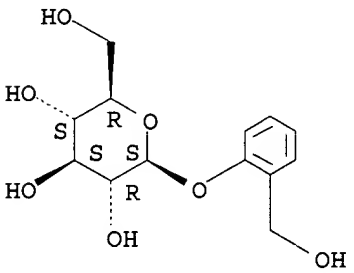
PRIORITY APPLN. INFO.: DE 2000-10034328 20000714

AB The invention concerns skin compns. that contain quercetin, rutin, salicin, and escin; escin is added as horse chestnut or wine leaf ext. The compns. are gels, emulsions, solns.,creams, suspension; they further contain thickening agents, preservatives. Thus a formulation contained (wt./wt.%): quercetin dihydrate 0.01; rutin trihydrate 0.010; D-(-)-salicin 0.010; escin 0.003; wine leaf ext. 0.425; glyceryl polyacrylate 10.00; sodium hydroxide 0.011; preservative 0.100; water to 100.

IT **138-52-3**, Salicin
RL: COS (Cosmetic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cosmetic and dermacol. compns. contg. quercetin, rutin, salicin, and escin)

RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:560508 CAPLUS
DOCUMENT NUMBER: 135:288062
TITLE: Does excretion of secondary metabolites always involve a measurable metabolic cost? Fate of plant antifeedant salicin in common brushtail possum, Trichosurus vulpecula
AUTHOR(S): McLean, S.; Pass, G. J.; Foley, W. J.; Brandon, S.; Davies, N. W.
CORPORATE SOURCE: School of Pharmacy, University of Tasmania, Hobart, 7001, Australia
SOURCE: Journal of Chemical Ecology (2001), 27(6), 1077-1089
CODEN: JCECD8; ISSN: 0098-0331
PUBLISHER: Kluwer Academic/Plenum Publishers

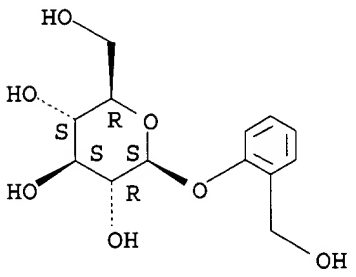
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Salicin was given to 6 brushtail possums in diet for 6 days at 0.05, 0.5, and 1.5% feed wet wt. (mean daily intakes 0.31.+-.0.09, 2.76.+-.0.75, and 6.04.+-.1.12 mmol salicin, resp.). Salicin metabolites were analyzed by HPLC and MS. Salicyl alc. glucuronide accounted for 56-64% of urinary metabolites over the 3 doses, salicyluric acid 15-26%, and salicin 10-18%; there were smaller amts. of free (2-4%) and conjugated (0-6%) salicylic acid. The .beta.,2-**dihydroxyphenylpropionic** acid was a minor metabolite. Hydrolysis of the dietary salicin allowed reconjugation of its aglycon, salicyl alc., with a more polar sugar, glucuronic acid, thus enhancing its renal excretion and leading to small net loss of substrates for conjugation and low measurable metabolic costs of excretion.

IT **138-52-3**, Salicin
RL: BPR (Biological process); BSU (Biological study, unclassified); FFD (Food or feed use); BIOL (Biological study); PROC (Process); USES (Uses)
(dietary salicin plant antifeedant compd. intake and metabolic cost of its urinary metabolites excretion in common brushtail possum (Trichosurus vulpecula))

RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:472959 CAPLUS
DOCUMENT NUMBER: 135:75834
TITLE: Enzyme-catalysed modification of substances in biological mixtures
INVENTOR(S): Otto, Ralf; Weiss, Albrecht
PATENT ASSIGNEE(S): Cognis Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046452	A1	20010628	WO 2000-EP12652	20001213
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
DE 19962204	A1	20010705	DE 1999-19962204	19991222
EP 1240349	A1	20020918	EP 2000-987394	20001213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				

PRIORITY APPLN. INFO.: DE 1999-19962204 A 19991222

WO 2000-EP12652 W 20001213

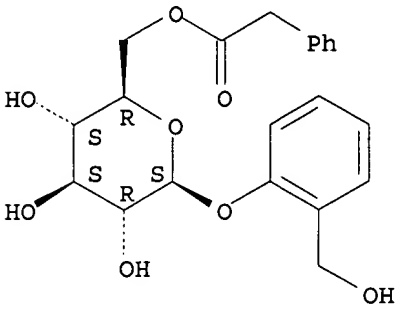
AB The invention relates to an enzyme-catalyzed modification of substances in a mixt., comprising bringing the substance in a mixt. to be modified into contact with an enzyme and a substrate. Thus, arbutin present in a com. leaf ext. of bearberry was mixed with palmitic acid in the presence of an immobilized lipase and incubated at 45 .degree.C for 24 h. The resulting palmitoyl arbutin was then extd. with chloroform or methylene chloride.

IT **270081-79-3P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(enzyme-catalyzed modification of compds. in biol. exts.)

RN 270081-79-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

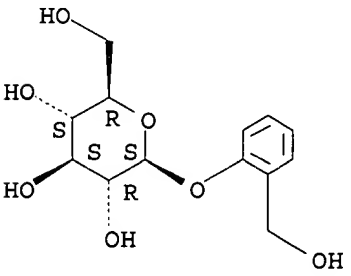


IT **138-52-3**, Salicin
RL: BOC (Biological occurrence); BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PROC (Process); RACT (Reactant or reagent)
(enzyme-catalyzed modification of compds. in biol. exts.)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:742053 CAPLUS

DOCUMENT NUMBER: 133:310142

TITLE: Synthesis, activity and formulations of pharmaceutical compounds for treatment of oxidative stress and/or endothelial dysfunction

INVENTOR(S): Del Soldato, Piero

PATENT ASSIGNEE(S): Nicox S.A., Fr.

SOURCE: PCT Int. Appl., 159 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000061537	A2	20001019	WO 2000-EP3234	20000411
WO 2000061537	A3	20010927		
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, DM, EE, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
IT 1311924	B1	20020320	IT 1999-MI753	19990413
BR 2000009702	A	20020108	BR 2000-9702	20000411
EP 1169294	A2	20020109	EP 2000-925203	20000411
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002541233	T2	20021203	JP 2000-610814	20000411
NO 2001004927	A	20011213	NO 2001-4927	20011010

PRIORITY APPLN. INFO.: IT 1999-MI753 A 19990413
WO 2000-EP3234 W 20000411

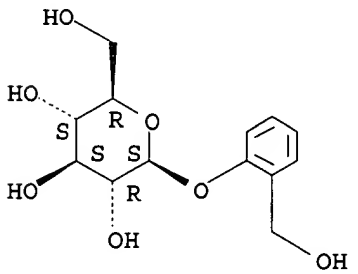
OTHER SOURCE(S): MARPAT 133:310142

AB Compds. A-B-C-N(O)s and A-C1[N(O)s]-B1 or their salts [s is an integer 1 or 2, preferably s = 2; A is the radical of a drug and is such as to meet the pharmacol. tests reported in the description; C and C1 are two bivalent radicals; the precursors of the radicals B and B1 are such as to meet the pharmacol. test reported in the description] were prepd. for use as pharmaceuticals. Thus, (S,S)-N-acetyl-S-(6-methoxy-.alpha.-methyl-2-naphthalenylacetyl)cysteine 4-nitroxybutyl ester was prepd. (NCX 2101) from naproxene and N-acetylcysteine in the first of 28 synthetic examples given. Pharmacol. test examples and tabular data are also given.

IT **138-52-3**, Salicin
RL: RCT (Reactant); RACT (Reactant or reagent)
(drug precursor)

RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



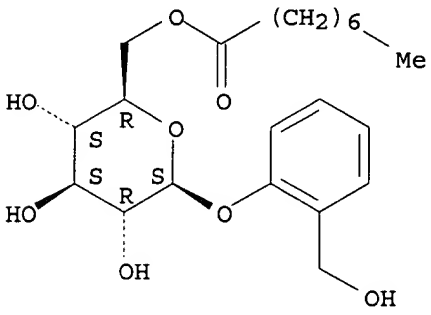
L13 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:155916 CAPLUS
DOCUMENT NUMBER: 132:344753
TITLE: Substrate specificity of lipase B from Candida antarctica in the synthesis of arylaliphatic glycolipids
AUTHOR(S): Otto, R. T.; Scheib, H.; Bornscheuer, U. T.; Pleiss,

J.; Syldatk, C.; Schmid, R. D.
CORPORATE SOURCE: Institut fur Technische Biochemie, Universitat Stuttgart, Stuttgart, D-70569, Germany
SOURCE: Journal of Molecular Catalysis B: Enzymatic (2000), 8(4-6), 201-211
CODEN: JMCEF8; ISSN: 1381-1177
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Arylaliph. glycolipids are known for their pharmaceutical and medicinal properties. We found that a great variety of arylaliph. esters can be synthesized from non-activated substrates such as glucose or the naturally-occurring drug salicin using lipase B from Candida antarctica (CAL-B). However, esters known to display anticancer activity such as those derived from arom. carboxylic acids or unsatd. arylaliph. acids, like cinnamic acid and its derivs., could not be obtained. In this work, along with syntheses of new glycolipids, we performed computer-aided mol. modeling based on data from our recently published work to examine why some substances are accepted by CAL-B while others are not. In order to elucidate the advantages and limitations of CAL-B in the synthesis of arom. glycolipids, we investigated arylaliph. acyl donor access to the lipase binding site along with steric interactions between the glucoside aglycons and residues of the alc. binding pocket.

IT **270081-72-6P 270081-75-9P 270081-77-1P**
270081-79-3P 270081-81-7P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(mol. modeling provides insight into substrate specificity displayed by Candida antarctica lipase B in synthesis of arylaliph. glycolipids)

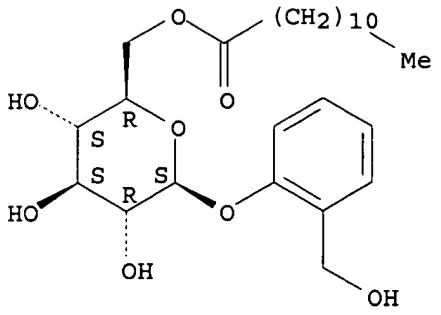
RN 270081-72-6 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-octanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



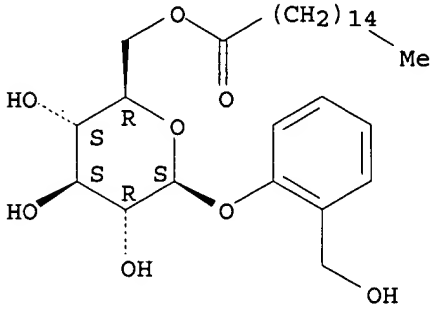
RN 270081-75-9 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-dodecanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



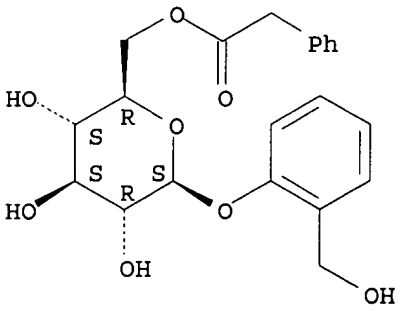
RN 270081-77-1 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-hexadecanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



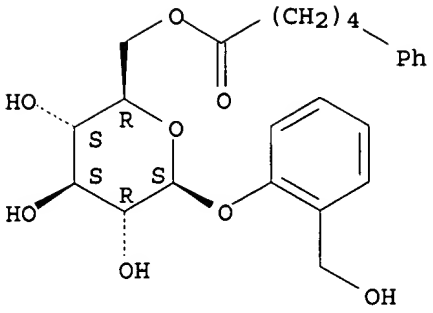
RN 270081-79-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzeneacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



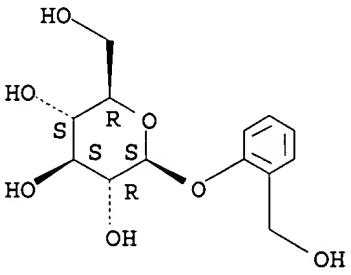
RN 270081-81-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenepentanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **138-52-3**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(mol. modeling provides insight into substrate specificity displayed by Candida antarctica lipase B in synthesis of arylaliph. glycolipids)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:393069 CAPLUS
DOCUMENT NUMBER: 131:43666
TITLE: Method for selective esterification of polyols
INVENTOR(S): Otto, Ralf; Syldatk, Christoph; Cao, Linqiu; Bornscheuer, Uwe; Schmid, Rolf D.
PATENT ASSIGNEE(S): Henkel K.-G.a.A., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19753789	A1	19990617	DE 1997-19753789	19971204

PRIORITY APPLN. INFO.: DE 1997-19753789 19971204
OTHER SOURCE(S): CASREACT 131:43666; MARPAT 131:43666
AB The prodn., from the corresponding polyol and carboxylic acid contg. an arom. ring, of polyols esterified on the primary -OH group is improved in selectivity and yield without introducing and removing protecting groups. This is characterized in that the polyol and carboxylic acid, in the presence of a small amt. of org. solvent that dissolves neither completely, react with each other under catalysis by a lipase or an

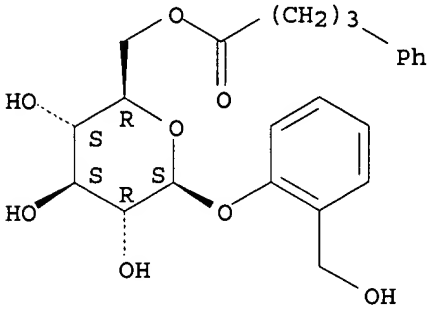
esterase. The products have emulsifying activity with potential pharmaceutical use.

IT **218966-96-2P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(selective esterification of polyols)

RN 218966-96-2 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzenebutanoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

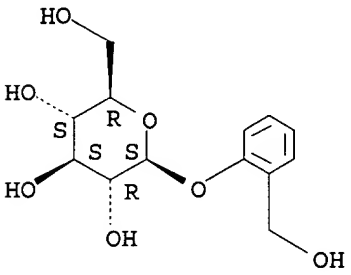


IT **138-52-3**, Salicin
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); PROC (Process); RACT (Reactant or reagent)
(selective esterification of polyols)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:653232 CAPLUS

DOCUMENT NUMBER: 127:326326

TITLE: Lowering effect of phenolic glycosides on the rise in postprandial glucose in mice

AUTHOR(S): Takii, Hiroshi; Matsumoto, Keitaro; Kometani, Takashi; Okada, Shigetaka; Fushiki, Tohru

CORPORATE SOURCE: Biochemical Research Laboratory, Ezaki Glico Co., Ltd., Osaka, 555, Japan

SOURCE: Bioscience, Biotechnology, and Biochemistry (1997), 61(9), 1531-1535
CODEN: BBBIEJ; ISSN: 0916-8451

PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

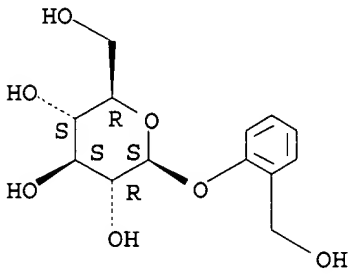
AB Glycosides were screened for their lowering effect on the postprandial blood glucose rise in vivo. The effect of phlorizin and other phenolic glycosides on the postprandial blood glucose response to glucose ingestion was evaluated in Std ddY mice. When phlorizin was simultaneously added, the peak blood glucose level was significantly decreased by 51% compared to vehicles following glucose ingestion by mice, while the blood insulin responses were generally similar. Screening expts. were conducted with different classes of phenolic glycosides added to a glucose soln. Redns. of 40-52% were obsd. in vehicles contg. arbutin, 4-**hydroxyphenyl** -.alpha.-D-glucopyranoside (hydroquinone-.alpha.-glucoside) or glycyrrhizin, and of only 15-31% (not significant) in vehicles contg. neohesperidin dihydrochalcone, glycyrrhetinic acid monoglucuronide, or 3,4-dimethoxyphenyl-.beta.-D-glucopyranoside. No lowering effect was obsd. in vehicles contg. salicin. Since glycyrrhizin, arbutin, and hydroquinone-.alpha.-glucoside blunted to varying degrees the postprandial blood glucose rise following glucose ingestion, they may be useful adjuvants for the treatment of diabetic subjects.

IT **138-52-3**, Salicin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lowering effect of phenolic glycosides on rise in postprandial glucose in mice in relation to diabetes treatment)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:106411 CAPLUS

DOCUMENT NUMBER: 126:140630

TITLE: Significance and application of microbial toxicity tests in assessing ecotoxicological risks of contaminants in soil and sediment

AUTHOR(S): van Beelen, P.; Doelman, P.

CORPORATE SOURCE: National Inst. Public Health Environment, Bilthoven, 3720 BA, Neth.

SOURCE: Chemosphere (1997), 34(3), 455-499
CODEN: CMSHAF; ISSN: 0045-6535

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Micro-organisms are vital for soil fertility and for the degrdn. of org. matter and pollutants in soils and sediments. Due to their function and ubiquitous presence micro-organisms can act as an environmentally very relevant indicator of pollution. Microbial tests should be used discriminatory for the establishment of soil and sediment quality guidelines. This review gives an evaluation of microbial toxicity tests and a novel method to derive quality guidelines. Long term microbial tests are generally less sensitive than short term tests. The toxic

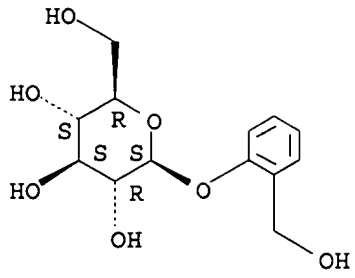
effects can be obscured by the activity of a few resistant micro-organisms, when for example soil respiration is used as a sum parameter during a long incubation period. Mineralization tests with high substrate concns. which enable growth, are less sensitive than similar tests with low concns. of substrate. The latter tests are more relevant for natural ecosystems. The often applied microbial toxicity tests can be categorized as single species tests, biomass measurements, carbon and nitrogen transformations, enzymic tests and tests measuring changes in microbial diversity. Comparisons between tests can only be indicative because the relative sensitivity depends on the toxicants and soils used. The respiration rate per unit of biomass is a more sensitive indicator of toxic effects than the respiration rate or the amt. of biomass alone. The autotrophic nitrification and acetylene redn. tests can be sensitive when short incubation times are used. The nitrogen mineralization, denitrification and many enzymic tests are often not very sensitive. The urease activity is a relatively sensitive enzymic test in many studies. The replacement of sensitive micro-organisms by different resistant species can have serious ecol. consequences. Some species become extinct while others appear in bulging nos. Adaptation of a community to a pollutant must be considered as the very process which disturbs a polluted ecosystem. The resistant micro-organisms often fail to perform specific ecol. functions. The occurrence of resistant species can be used as an sensitive and ecol. relevant indicator for deterioration from environmental pollution. Persistent toxic effects on the microflora can be caused by zinc, cadmium and copper at concn. levels lower than European Community limits. Tests with anaerobic sediment processes were orders of magnitude more sensitive for some chlorinated aliph. compds. than aquatic toxicity tests. The addn. of a few mg zinc per kg soil can inhibit the more sensitive microbial processes (like chloroform or 4-chlorophenol degrdn.), whereas soil invertebrates and some plants are less sensitive to zinc. After the evaluation of the tests, a novel method is described to derive soil and sediment quality guidelines using microbial toxicity tests. The results of single species tests with micro-organisms can be incorporated into the contemporary risk assessment method for higher organisms which is based on the extrapolation from single species tests to the protection of 95% of all species in an ecosystem. This method uses the No Obsd. Effect Concns. (NOEC) of a no. of toxicity tests to calc. a Hazardous Concn. 5% (HC5). The HC5 is calcd. from more than 5 NOEC values. In analogy the Effect Concn. 10% (EC10) can be used to calc. the Dangerous Concn. 5% (DC5). The DC5 is calcd. from more than 5 EC10 values. The DC5 should give protection to 95% of the microbial processes. The DC5 of a no. of pollutants are calcd. and compared with the HC5 values from the literature. Microbial toxicity tests can be used for risk assessment because micro-organisms are among the most sensitive organisms for the effects of pollutants.

IT **138-52-3**, Salicine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(application of microbial toxicity tests in assessing ecotoxicol. risks of contaminants in soil and sediment)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



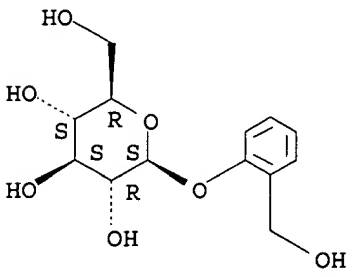
L13 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:481839 CAPLUS
DOCUMENT NUMBER: 121:81839
TITLE: Effects of heavy metals in soil on microbial diversity and activity as shown by the sensitivity-resistance index, an ecologically relevant parameter
AUTHOR(S): Doelman, P.; Jansen, E.; Michels, M.; van Til, M.
CORPORATE SOURCE: IWACO B.V., Rotterdam, 3009 AM, Neth.
SOURCE: Biology and Fertility of Soils (1994), 17(3), 177-84
CODEN: BFSOEE; ISSN: 0178-2762
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A sensitivity-resistance index was developed, and proved to be a very sensitive biomonitor of soil pollution with heavy metals. The index was developed by a step-by-step approach. Ultimately, the bacterial soil microflora was divided into three groups, sensitive, tolerant, and resistant microflora. Zn and Cd sensitivity was defined as no growth occurring in the presence of 5 and 0.5 mg L-1 of these metals, resp., while resistance was defined as distinct growth in the presence of 50 and 16 mg L-1, resp. The sensitivity:resistance ratio of a ref. clay soil (0.57 mg Cd kg-1 and 140 mg Zn kg-1) was 0.53, but for polluted (6 mg Cd kg-1 + 670 mg Zn kg-1) clay soil, the ratio was 0.24. For a ref. (0.06 mg Cd kg-1 + 12 mg Zn kg-1) sandy soil, the sensitivity:resistance ratio was 1.50 whereas polluted (2.3 mg Cd kg-1 + 252 mg Zn kg-1) sandy soil had a ratio 0.19. The ecol. value of the sensitivity-resistance lies in its capacity to reflect potential degrdn. of arom. compds. It has been shown repeatedly that sensitive bacteria grow significantly better on a range of selected arom. compds. It has been speculated that resistance to heavy metals may reduce the bioremediation capacity of soil towards chlorinated aroms. and polyarom. hydrocarbons.

IT **138-52-3**, Salicine
RL: BIOL (Biological study)
(soil microorganism growth on, sensitivity and resistance to heavy metal contamination in relation to)

RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



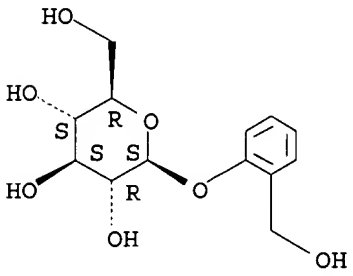
L13 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:228730 CAPLUS
DOCUMENT NUMBER: 120:228730
TITLE: Materials science of organic compounds. Part 3. Glass-formers, vitriphores, Tg, and molecular chirality
AUTHOR(S): Tiers, George V. D.
CORPORATE SOURCE: 3M Corporate Research Laboratories, 201-2S-14, Box 33221, St. Paul, MN, 55133, USA
SOURCE: Thermochimica Acta (1993), 226(1-2), 317-24
CODEN: THACAS; ISSN: 0040-6031
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Various chiral p-nitrophenylurethanes and ureas, useful for SHG, were studied by DSC. On quench-cooling from the melt, these compds. invariably formed glasses and gave glass-transition temps. (Tg) values on reheating. This behavior was generalized, first to other homochiral compds., and then to racemic mixts. For mixts. the Tg values were not strictly linear interpolations.The rule is proposed that mol. chirality, even when of steric origin and/or rapidly inverting, strongly favors glass formation. An attached dissym. group is termed a "vitriphore".

IT **138-52-3**, Salicin
RL: PRP (Properties)
(thermal properties of, DSC study of)

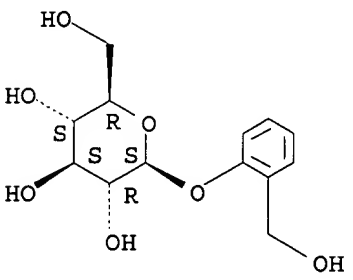
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:468768 CAPLUS
DOCUMENT NUMBER: 115:68768
TITLE: Identification by gas chromatography-mass spectrometry of 150 compounds in propolis
AUTHOR(S): Greenaway, W.; May, J.; Scaysbrook, T.; Whatley, F. R.
CORPORATE SOURCE: Dep. Plant Sci., Univ. Oxford, Oxford, OX1 3RB, UK
SOURCE: Zeitschrift fuer Naturforschung, C: Journal of Biosciences (1991), 46(1-2), 111-21
CODEN: ZNCBDA; ISSN: 0341-0382
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Propolis was analyzed by gas chromatog.-mass spectrometry for both its headspace volatiles and for the less volatile components of its alc. ext. (propolis balsam). One hundred eighty-one peaks were located of which 171 representing 150 compds. were identified, including 28 identified in propolis for the first time. The majority of compds. were typical of poplar bud exudate.
IT **138-52-3**, Salicin
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of propolis from honeybee hives)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

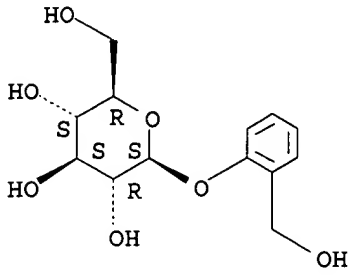
Absolute stereochemistry.



L13 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:92090 CAPLUS
DOCUMENT NUMBER: 110:92090
TITLE: Phenolic analysis of bud exudate of Populus lasiocarpa by GC/MS
AUTHOR(S): Greenaway, W.; Scaysbrook, T.; Whatley, F. R.
CORPORATE SOURCE: Dep. Plant Sci., Oxford, OX1 3RA, UK
SOURCE: Phytochemistry (1988), 27(11), 3513-15
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The summer bud exudate of two plants of P. lasiocarpa analyzed by GC/MS lacked the flavonoid aglycons and substituted benzoic and phenolic acid esters characteristic of other poplar species. Other compds., such as syringaldehyde, syringic acid, and shikimic acid, not previously identified in bud exudate of other poplar species were found, as were catechin, catechol, quinic acid, and salicin, compds. not normally present in poplar bud exudate. The exudates from the two sources differed considerably in detailed compn.
IT **138-52-3**, Salicin
RL: BIOL (Biological study)
(in bud exudate of poplar)
RN 138-52-3 CAPLUS

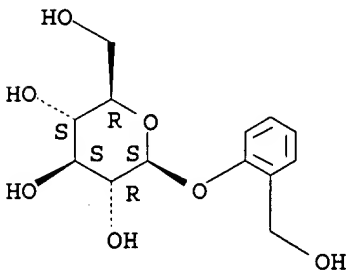
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:78258 CAPLUS
DOCUMENT NUMBER: 106:78258
TITLE: Comparison of calculated versus measured partition coefficients of some phenyl .beta.-D-glucopyranosides
AUTHOR(S): Kim, Ki Hwan; Martin, Yvonne C.
CORPORATE SOURCE: Abbott Lab., North Chicago, IL, 60064, USA
SOURCE: Journal of Pharmaceutical Sciences (1986), 75(7), 637-8
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Exptl. detd. octanol [111-87-5]-water partition coeff. values of substituted Ph .beta.-D-glucopyranosides are compared with the calcd. values using the computer program CLOGP. The systematic deviation of the calcd. values from the measured ones in this series suggests that caution is required when calcns. are performed on classes of compds. where many of the partition coeffs. have not been exptl. detd.
IT **138-52-3**
RL: PRP (Properties)
(partition coeffs. of, calcd. vs. measured)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

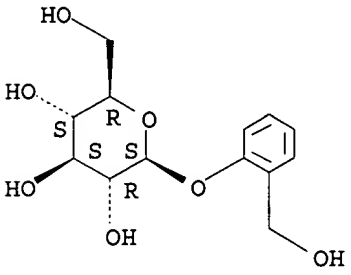
Absolute stereochemistry.



L13 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1975:121674 CAPLUS
DOCUMENT NUMBER: 82:121674
TITLE: Phenolic compounds of Salix alba X babylonica bark
AUTHOR(S): Kompantsev, V. A.; Gaidash, P. M.; Dauksha, A. D.
CORPORATE SOURCE: Pyatigorsk. Farm. Inst., Pyatigorsk, USSR
SOURCE: Khimiya Prirodnykh Soedinenii (1974), (6), 807-8
CODEN: KPSUAR; ISSN: 0023-1150

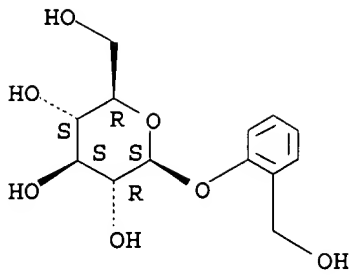
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB 3-(4-**Hydroxyphenyl**)-2-propenyl-1-O-.beta.-D-glucopyranoside (triandrin) and saligenin-2-O-.beta.-D-glucopyranoside (salicin) were identified after sepn. by column chromatog. on cellulose of compds. crystd. from the purified water ext. of the bark. Chromatog. on paper revealed the presence in the ext. of (.+-.)-gallocatechol, (.+-.)-catechol, (-)-epigallocatechol gallate, and epicatechol gallate.
IT **138-52-3**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of willow bark)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1970:51645 CAPLUS
DOCUMENT NUMBER: 72:51645
TITLE: Fluorometric determination of carbohydrates
AUTHOR(S): Guilbault, George G.; Sadar, M. H.; Peres, K.
CORPORATE SOURCE: Louisiana State Univ., New Orleans, LA, USA
SOURCE: Analytical Biochemistry (1969), 31, 91-101
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Fluorometric methods are described for the detn. of hexokinase and .beta.-glucosidase, and glucose, fructose, maltose, cellobiose lactose, glycogen, and salicin. Glucose and fructose are detd. fluorometrically by using hexokinase and the resazurin-resorufin indicator reaction G. G. G. and D. N. Kramer , 1965. Maltose, cellobiose, lactose, glycogen, and salicin are enzymically hydrolyzed to glucose, which is then detd. fluorometrically by using glucose oxidase, p-**hydroxyphenylacetic** acid, and peroxidase. All the carbohydrates were assayed in the range 0.01-50 .mu.g/ml and the enzymes hexokinase and .beta.-glucosidase in the range 10-3 to 10-1 unit/ml with an error and precision of about 1.5%.
IT **138-52-3**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, fluorimetric)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

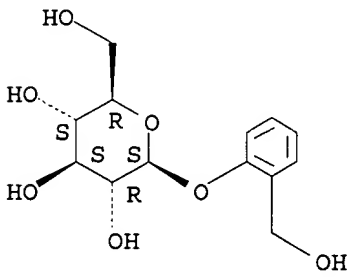


L13 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1968:493644 CAPLUS
DOCUMENT NUMBER: 69:93644
TITLE: Leaves of the family Salicaceae. XI. The hot water extractives of the leaves of Populus balsamifera
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Phytochemistry (Elsevier) (1968), 7(10), 1845-9
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The hot water extractives of fresh leaves from P. balsamifera trees cut in May and in September were extd. fractionally with EtOAc, and the EtOAc exts. were fractionated by elution chromatog. with water on a polyamide column. Cryst. compds. isolated were salicin, salicyl alc., pyrocatechol, (-)-3-hydroxy-5-phenyl-valeric acid (I), trichocarpin, cinnamic acid, and p-coumaric acid. Yields of all identified products were much smaller in the September than in the May leaves. This is the first report of cinnamic acid, p-coumaric acids, and I in the leaves of any Populus species and the first report of I in any plant source.

IT **138-52-3**
RL: BIOL (Biological study)
(in Populus balsamifera leaves)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1968:441265 CAPLUS
DOCUMENT NUMBER: 69:41265
TITLE: The hydrophobic character of phenyl glycosides and its relation to the binding of saccharides to concanavalin A
AUTHOR(S): Poretz, R. D.; Goldstein, I. J.
CORPORATE SOURCE: Univ. of Michigan, Ann Arbor, MI, USA
SOURCE: Archives of Biochemistry and Biophysics (1968), 125(3), 1034-6

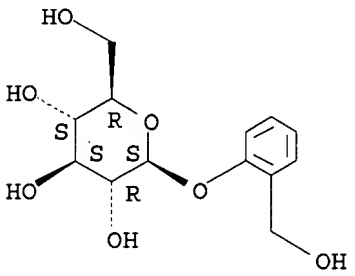
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Recent studies (R. D. Poretz and I. J. Goldstein, 1967) suggested the presence of a region on the concanavalin A mol., the jack bean hemagglutinin, adjacent to the specific saccharide binding site, which is capable of interacting specifically with the aromatic moiety of phenyl .beta.-D-glucopyranosides. In an effort to elucidate the mode of interaction between the protein and the aglycon of the bound saccharide, the authors exptl. detd. .pi. (a parameter indicative of the hydrophobicity of an atom or group of atoms) for a variety of aryl-substituted phenyl .beta.-D-glycopyranosides. The data show that .pi. is indeed a const. indicative of the properties of the substituent and relatively independent of the remainder of the mol. The .pi. value for a mol. contg. multiple substituents is apparently equiv. to the sum of the .pi. values for the individual substituents. These data are consistent with the hypothesis that concanavalin A possesses an apolar region, adjacent to the polar saccharide binding site, which is capable of interacting specifically with the meta, but not para, portion of aromatic nuclei joined directly to the .beta.-glycosidic O atom, presumably by means of hydrophobic forces.

IT **138-52-3**
RL: PRP (Properties)
(hydrophobic substituent const. of, concanavalin A hydrophobic binding site in relation to)

RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

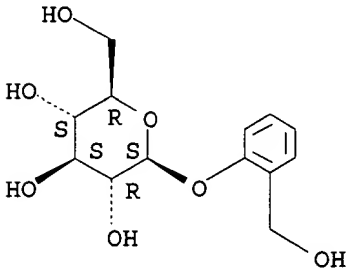


L13 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:29040 CAPLUS
DOCUMENT NUMBER: 66:29040
TITLE: Action of bromine water on some phenolic glucosides
AUTHOR(S): Moreno, Alcira; Cardini, Carlos E.
CORPORATE SOURCE: Fac. Cienc. Exactas Nat., Buenos Aires, Argent.
SOURCE: Anales de la Asociacion Quimica Argentina (1965), 53(3-4), 269-76
CODEN: AAQAAE; ISSN: 0365-0375
DOCUMENT TYPE: Journal
LANGUAGE: Spanish

AB A soln. of 1-2 .mu.m./ml. of arbutin (I) is treated with a few drops of Br water until a very light yellow coloration appears. The soln. is immediately aerated. Paper chromatog. (Whatman no. 1, 6:4:3 BuOH-C5H5N-H2O shows the disappearance of I and immediate and quant. formation of D-glucose. The uv spectrum of the soln. is that of p-benzoquinone with no I remaining. The related p-methoxy and p-ethoxyphenyl glucosides, p-**hydroxyphenyl** cellobiose and gentiobiose give the same results. With m-hydroxy phenyl glucoside an excess of Br water is needed and the reaction takes place through the formation of resorcinol Br derivs.

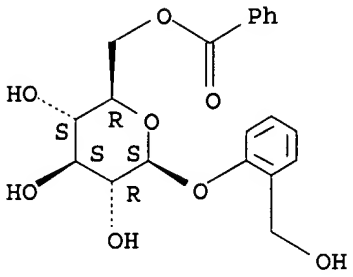
IT **138-52-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with bromine water)
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:475361 CAPLUS
DOCUMENT NUMBER: 65:75361
ORIGINAL REFERENCE NO.: 65:14106f-h,14107a
TITLE: Dark fixation of carbon dioxide by healthy and rust-affected leaves of wheat and bean
AUTHOR(S): Daly, J. M.; Livne, A.
CORPORATE SOURCE: Univ. of Nebraska, Lincoln
SOURCE: Phytopathology (1966), 56(2), 164-9
CODEN: PHYTAJ; ISSN: 0031-949X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. following abstr. A quant. comparison was made of the ability of rust-affected and healthy leaves of bean (Phaseolus vulgaris) and wheat (Triticum aestivum) to fix CO2 in the dark. Methods were compared for supplying radioactive CO2 in the atm. or in solns. bathing the tissue. With both methods, marked diurnal changes in capacity to fix CO2 into org. compds. were observed. At the end of a dark period, tissues fixed less CO2 than after exposure to light for several hrs. When CO2 was supplied from the atm., there was no significant difference between healthy and rust-affected tissue until sporulation occurred; then, diseased tissue fixed more CO2 than did healthy tissue, but only at the end of a dark period, probably because rupture of the epidermis compensated for stomatal closure in the dark. From soln., much more CO2 was fixed by both types of tissue, but diseased tissue was markedly inhibited after sporulation was initiated, and the inhibition was independent of diurnal fluctuations. Calcns. that magnify the role of dark CO2 fixation for diseased tissue indicate that it is unlikely that dark fixation of CO2 is of quant. significance in the accumulation of org. compds. in rust-affected tissue. In order to examine the metabolic mechanisms that caused reduced dark CO fixation from solns. by diseased tissue, fractionation of tissue components was made. Nearly all of the 14C fixed appeared in the org. acid fraction. Malic and aspartic acids were the primary acids formed, suggesting that isocitric dehydrogenase is not the system for CO2 fixation in rust-affected tissue. The relation between the amts. of malate and aspartate formed in healthy and diseased tissue suggests that levels of reduced pyridine nucleotides may be responsible for lower rates of formation of org. acids by dark CO2 fixation in rusted leaves.
IT **99-17-2**, Salicin, 6'-benzoate
(in broad bean, transport of)
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:475360 CAPLUS
DOCUMENT NUMBER: 65:75360
ORIGINAL REFERENCE NO.: 65:14106e-f
TITLE: Translocation of phenolic compounds
AUTHOR(S): Macleod, Norma J.; Pridham, J. B.
CORPORATE SOURCE: Roy. Holloway Coll., Univ., London
SOURCE: Phytochemistry (Elsevier) (1966), 5(4), 777-81
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English

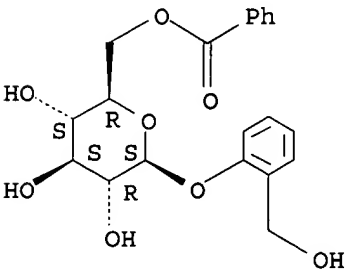
AB m-**Hydroxyphenyl**-.beta.-D-glucoside, arbutin, esculin, salicin, resorcinol, catechol, phloroglucinol, quinol, saligenin, caffeic acid, ferulic acid, kempferol, and quercetin applied to the epidermal surfaces of the laminae of Vicia faba became distributed over the entire plant, including the roots. The aphid stylet technique using Macrosiphum pisi feeding on V. faba stems and Tuberolachnus salignus feeding on Salix daphnoides clearly showed that phenols introduced into the leaves can move down the plant by the normal processes of translocation and there was definite evidence for the occurrence of phenolic compds. as natural constituents of sieve tubes. Tyrosine was found in sieve tubes of S. daphnoides.

IT **99-17-2**, Salicin, 6'-benzoate
(in broad bean, transport of)

RN 99-17-2 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:29217 CAPLUS
DOCUMENT NUMBER: 64:29217
ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b
TITLE: Leaves of the family Salicaceae. V. The occurrence of

glucosides in the leaves of Populus grandidentata

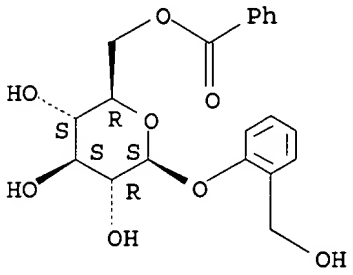
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Tappi (1965), 48(10), 607-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of P. grandidentata, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H2O and the granular ppt. filtered off. Extn. of the filtrate with Et2O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl3 and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H2O, the ppt. decompd. with H2S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H2O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H2O and 7 ml. concd. H2SO4 in 100 ml. H2O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin benzoate (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H2O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et2O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

IT **99-17-2**, Populin **138-52-3**, Salicin **529-66-8**, Tremuloidin
(in poplar leaves)

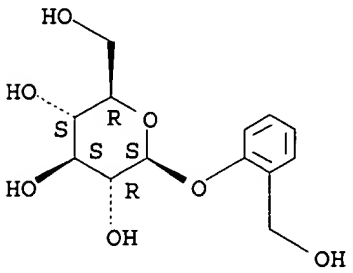
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



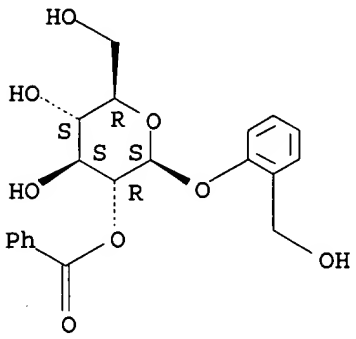
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



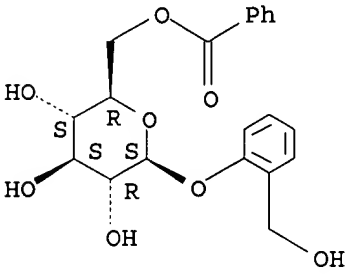
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **99-17-2**, Populin
(salicylate, in popular leaves)
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1964:400290 CAPLUS
DOCUMENT NUMBER: 61:290
ORIGINAL REFERENCE NO.: 61:41a-b
TITLE: Detection of nonreducing carbohydrate compounds with complex cuprates(III)
AUTHOR(S): Kocourek, J.; Ticha, M.; Kostir, J.; Jensovsky, L.
CORPORATE SOURCE: Karlova Univ., Prague
SOURCE: Journal of Chromatography (1964), 14(2), 228-31
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Nonreducing carbohydrates are detected on paper chromatograms with K telluratocuprate(III). The descending technique was employed, using Whatman No. 1 or No. 3 filter paper in 10:1:3 BuOH-AcOH-H2O except in the case of the higher oligosaccharides where 6:3:1 PrOH-NH4OH-H2O was used. The sugar compds. give white spots on a distinctive deep yellow-brown background. The background disappears after a few min. The unsubstituted sugars, glycosides, glycosans, and anhydrosugars are detectable in amts. of 1 .gamma.. In substituted sugars, e.g. in fully acylated sugars easily hydrolyzable in a strong alk. medium, or in various alkylidene derivs. with at least 1 pair of vicinal hydroxyl groups, the sensitivity is 5-10 .gamma.. The non-reactive substances include the alkali stable polytopic

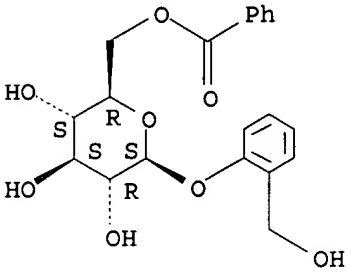
alkylidene and arylidene derivs., such as the various di- and tribenzylidene or isopropylidene derivs. of monoses and glycitols.

IT **99-17-2**, Salicin, 6'-benzoate
(detn. on paper chromatograms)

RN 99-17-2 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1962:7859 CAPLUS

DOCUMENT NUMBER: 56:7859

ORIGINAL REFERENCE NO.: 56:1518a-i

TITLE: Dealkylation and deacylation of carbohydrate derivatives with boron trichloride and boron tribromide

AUTHOR(S): Bonher, T. G.; Bourne, E. J.; McNally, S.

CORPORATE SOURCE: Univ. London

SOURCE: Journal of the Chemical Society, Abstracts (1960) 2929-34
CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Use of BCl3 (I) and BBr3 (Ia) for deacylating esters and demethylating Me ethers of carbohydrates was described; derivs. of di- and polysaccharides were hydrolyzed to their monosaccharide components. DFructose (II) and L-sorbose (III) were degraded to 5-(hydroxymethyl)-2-furaldehyde (IV), but all other monosaccharides studied were stable to the reagents. The carbohydrate deriv. (1-10 mg.) was suspended or disssolved in 1-2 ml. anhyd. CH2Cl2 and cooled in dry ice-Me2CO, 1-2 g. I added at -80.degree., the mixt. kept 30 min. at -80.degree. and 16 hrs. at room temp., solvent and I removed by evapn., and the glassy residue treated (a) with three 3-ml. portions MeOH with evapn. after each addn., or (b) with Ag2CO3H2O to neutrality, followed by filtration and freeze-drying of the filtrate. Either residue was then dissolved in MeOH or H2O and the soln. examd. by papergrams and paper ionophoresis. Thus the following were prepd. [starting compd., major product, trace product(s)]: 2,3,5-trimethyl ether of L arabinose (V), V, oligosaccharides (VI) of Rf 2.7 and 3.8 in 4:1:5 BuOH-EtOH-H2O (VII); 2,4-dimethyl ether of V, V, material Rf 1.4; 2-Me ether (VIII) of L-fucose (IX), IX, VI and VIII; Me 2,3,4-tri-O-methyl-L-fucoside, IX, material Rf 0.9; 2,3,4,6-tetramethyl ether of D-galactose (X), X, material Rf 0.88; 3,4-dimethyl ether of L-rhamnose (XI), XI, material Rf 0.88; 2,3,4,6-tetramethyl ether (XII) of D-glucose (XIII), XIII, mono- (XIV), di- (XV), and trimethyl ethers of XIII; 2,3,6-trimethyl ether of XIII, XIII, XIV and XV, RXII 0.77; Me 2,3-di-O-methyl-.alpha.-D-glucoside, XIII, XIV; 3-Me ether (XVI) of XIII, XIII, XVI; 2,3,4,6-tetramethyl ether of D-mannose (XVII), XVII, materials of RXII 0.37, 0.52, 0.61, 0.74, 0.93; 3,4-dimethyl ether of XVII (hydrate), XVII, materials RXII 0.40, 0.56; dimethyl ethers (XVIII) of sucrose, XIII and IV, II and XVIII; 3-Me ether of D-xylose (XIX), XIX, -; methyl ethers of

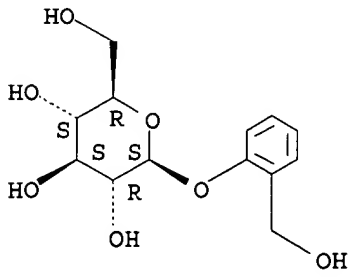
amylopectin (XX), XIII, XIV and XV; methyl ethers of cellulose (XXI), XIII, XIV and XV; Me .beta.-D-arabinoside (XXII), D-arabinose, XXII; Me .alpha.-D-fructofuranoside, II and IV, -; Me .alpha.-D galactoside, X, -; Me .beta.-D-galactoside, X, -; Me .alpha.-Dglucoside (XXIII), XIII, VI; Me .beta.-D-glucoside, XIII, -; Ph .alpha.-D-glucoside, XIII and PhOH, -; Ph .beta.-D-glucoside, XIII and PhOH, -; arbutin, XIII and hyroquinone, -; salicin, XIII and saligenin, -; Me .alpha.-D-mannoside (XXIV), XVII, VI; Me .alpha.-L-rhamnoside, XI, -; Me .beta.-D-riboside, Dribose (XXV), -; Me .alpha.-D-xylofuranoside, XIX, -; 4,6-O-benzylidene-D-glucose, XIII, -; 4,6-O-benzylidene acetal of XXIII, XIII, -; 1,2:5,6-di-O-isopropylidene-D-glucose, XIII, -; 1,2-O-isopropylidene-D-glucofuranose, XIII, -; 2,3:4,5-di-O-isopropylidene-D-fructose, IV, II; octaacetate of gentiobiose (XXVI), XIII, XXVI, Rf 1.15, Rf 1.5 in 7:1:2 PrOH-EtOAc-H2O; penta-O-acetyl-.beta.-D-glucose, XIII, materials of Rf 2.7 and 5.0; octa-O-acetylsucrose, XIII and IV, material of Rf 2.4; acetylated XX, XIII, VI of Rf 1.9 and 2.2; acetylated XXI, XIII, VI of Rf 1.9 and 2.2; 1,6-anhydro-.beta.-D-galactopyranose, X, VI; 1,6-anhydro-.alpha.-D-galactofuranose, X, VI; 1,6-anhydro-.beta.-D-glucopyranose, XIII, VI; 1,6-anhydro-.beta.-D-gulopyranose, D-gulose, VI; 1,6-anhydro-.beta.-D-mannopyranose, XVII, VI; 2,3-anhydro-4,6-O-benzylidene deriv. of XXIV, materials of RXVII 2.3 and 2.5, material of RXVII 4.7; Me 2,3-anhydro-.beta.-L-ribose, materials of RXXV 0.7 and 1.7, -; V, V, VI of RXIII 2.4; X, X, -; XIII, XIII, -; D-lyxose, D-lyxose, -; XVII, XVII, -; XI, XI, -; XIX, XIX, -; II, IV, material of Rf 0.90; III, IV, III; Ia + lactose, X and XII, lactose; Ia + maltose, XIII, maltose; Ia + melibiose, X and XIII, melibiose and material of RXIII 1.6; Ia + sucrose, XIII and IV, sucrose; Ia + turanose, XIII and IV, II; Ia + raffinose, X and XIII and IV, II; inulin, IV, --; nitrate ester of XXI, XII, materials of Rf 0.38, 2.1, and 3.6; 4,6-O-benzylidene-2,3-di-O-methyl deriv. of XXIII, XIII, XIV and XV and material of RXII 0.70; 4,6-O-benzylidene-2-O-(p-tolylsulfonyl) deriv. of XXIII, material of RXIII 5.7, XIII. The last result indicated that the p-tolylsulfonyl group was not hydrolyzed.

IT **138-52-3**, Salicin
(reaction with B halides)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1961:38216 CAPLUS

DOCUMENT NUMBER: 55:38216

ORIGINAL REFERENCE NO.: 55:7494c-d

TITLE: Reaction of carbohydrases with phenolic glucosides

AUTHOR(S): Anderson, J. D.; Hough, L.; Pridham, J. B.

CORPORATE SOURCE: Univ. Bristol, UK

SOURCE: Biochemical Journal (1960), 77, 564-7
CODEN: BIJOAK; ISSN: 0264-6021

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The incubation of almond emulsin, or enzyme prepns. from broad bean, with

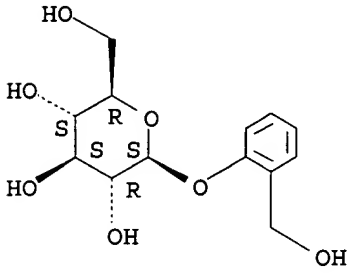
arbutin produces p-**hydroxyphenyl**-.beta.-gentiobioside. A transglucosylation reaction catalyzed by .beta.-glucosidase is involved with arbutin mols. serving as both donors and acceptors of D-glucopyranosyl residues. Salicin is partially converted to o-hydroxybenzyl-.beta.-glucopyranoside by the almond and broad-bean prepns.

IT **138-52-3**, Salicin
(hydrolysis of carbohydrases)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1960:86947 CAPLUS

DOCUMENT NUMBER: 54:86947

ORIGINAL REFERENCE NO.: 54:16549h-i

TITLE: Biosynthesis of plant glycosides. II. Gentiobiosides

AUTHOR(S): Yamaha, Tsutomu; Cardini, Carlos E.

CORPORATE SOURCE: Inst. Investigaciones Bioquim., Buenos Aires

SOURCE: Archives of Biochemistry and Biophysics (1960), 86, 133-7
CODEN: ABBIA4; ISSN: 0003-9861

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

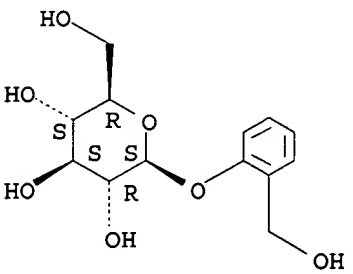
AB An enzyme from wheat germ which catalyzes the reaction, UDPG + phenol-.beta.-glucoside .fwdarw. UDP + phenol-.beta.-gentiobioside, has been purified and sepd. from the enzyme that catalyzes the formation of glucosides. The enzyme is specific for phenol-.beta.-glucosides, and catalyzes the addn. of only one glucose residue. Free sugars, disaccharides, or polysaccharides were not used for substrates. The rate of reaction decreased in the order: phenol glucoside > salicin > arbutin > p-methoxyphenol glucoside > m-methoxyphenol glucoside > resorcinol glucoside > mandelonitrile glucoside.

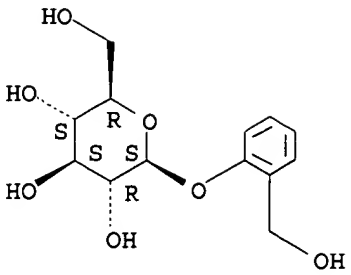
IT **138-52-3**, Salicin
(phenol-.beta.-gentiobioside formation from, by enzyme from wheat germ)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.





L13 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1959:14750 CAPLUS
DOCUMENT NUMBER: 53:14750
ORIGINAL REFERENCE NO.: 53:2735e-i,2736a-d
TITLE: Paper chromatography and paper electrophoresis of phenols and glycosides
AUTHOR(S): Coulson, C. B.; Evans, W. C.
CORPORATE SOURCE: Univ. Coll. North Wales, Bangor
SOURCE: Journal of Chromatography (1958), 1, 374-9
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The following Rf values and spot colorations with diazotized p-nitroaniline spray were obtained by ascending chromatography on Whatman No. 4 paper with C6H6-AcOH-H2O (20:5:satn.) (solvent A) and BuOH-EtOH-borate buffer (9.54 g. Na2B4O7/1.) (1:1:1) (solvent B), resp.: pyrocatechol 0.43, cherry purple, 0.70, brown; homocatechol 0.56, red-purple, 0.72, brown-red; phloroglucinol. 0.00, yellow-orange, 0.87, reddish mustard yellow; resorcinol 0.12, yellow-orange, 0.94, mustard yellow; saligenin 0.62, crimson, 0.74, brown-yellow; 8-quinolinol 0.60, purple, -, -; 3,4-dihydroxy-.omega.-chloroacetophenone 0.21, pale yellow, 0.62, yellow; dinitrophenylglycine 0.71, -, 0.70, -; dinitrophenylethanolamine 0.88, -, 0.90, -; .omicron.-HOC6H4CO2H 1.00, bright red, 0.74, yellow-red; m-HOC6H4CO2H 0.50, scarlet, 0.68, red; p-HOC6H4CO2H 0.42, light crimson, 0.65, red; .omicron.-HOC6H4CH2CH2CO2H 0.70, mauve, 0.79, red-mauve; m-HOC6H4CH2CH2CO2H 0.55, pink, 0.76, bright crimson; p-HOC6H4CH2CH2CO2H 0.53, blue-purple, 0.73, blue-purple; cis-o-HOC6H4CH:CHCO2H -, -, 0.81, purple; trans-.omicron.-HOC6H4CH:CHCO2H 0.65, bluish mauve, 0.74, purple; m-HOC6H4CH:CHCO2H 0.53, crimson, 0.70, crimson; p-HOC6H4CH:CHCO2H 0.50, bright blue, 0.66, blue-gray; o-**hydroxyphenylglyoxylic** acid 0.22, salmon, 0.83, salmon; p-**hydroxyphenylpyruvic** acid 0.44, purple, 0.70, purple; 2,3-(HO)2C6H3CO2H 0.43, cherry purple, 0.49, pale brown; 2,4-(HO)2C6H3CO2H 0.30, brown-mustard, 0.53, reddish brown; 2,5-(HO)2C6H3CO2H 0.20, yellow, 0.55-0.85, pale reddish brown; 2,6-(HO)2C6H3CO2H 0.16, yellow, 0.78, brown-gray; 3,4-(HO)2C6H3CO2H 0.08, cherry red, 0.30, brown; 3,5-(HO)2C6H3CO2H 0.02, bright yellow, 0.54, yellow; 2,3-(HO)2C6H3CH2CO2H 0.15, cherry purple, -, -; 2,5-(HO)2C6H3CH2CO2H (I) 0.03, brown, 0.65, white; 3,4-(HO)2C6H3CH2CO2H 0.05, cherry red, 0.39, light brown; 2,3-(HO)2C6H3CH2CH2CO2H 0.28, cherry purple, 0.45, medium orange; 2,5-(HO)2C6H3CH2CH2CO2H 0,09, brown, -, -; 3,4-(HO)2C6H3CH2CH2CO2H 0.13, cherry red, 0.42, quenched red; 2,5-(HO)2C6H3CH:CHCO2H 0.04, yellow, 0.4-0.6, pale brown; 3,4-(HO)2C6H3CH:CHCO2H 0.08, brownish purple, 0.40, gray-brown; 3,1,2-HOC6H3(CO2H)2, none, -, none; 4,1,2-HOC6H3(CO2H)2 0.02, bright crimson, 0.41, red; 3,4,1,2,(HO)2C6H2(CO2H)2 0.02, red, 0.20, quenched orange; 4,5,1,2-(HO)2C6H2(CO2H)2 0.01, pink, -, -; I lactone 0.03, light brown, streak, brown; 2,5-**dihydroxyphenylpyruvic** acid lactone 0.20, yellow-orange, 0.79, mustard yellow; 2,5-(HO)2C6H3CHO 0.63, pale yellow, 0.93, white; 3,4-(HO)2C6H3CHO 0.13, pale yellow, 0.62, white. Results were obtained in 8 and 18 hrs., resp., with solvents A and B. Sugars and related compds., chromatographed on paper buffered with

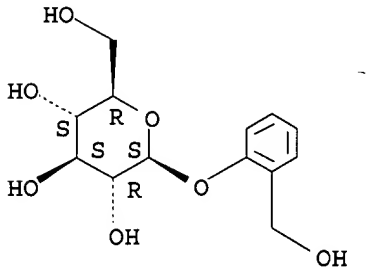
borate buffer, with solvent B and alk. AgNO3 to detect the spots, showed the following Rf values: arabinose 0.22, arbutin 0.72, ascorbic acid 0.28, erythritol 0.27, fructose 0.23, fucose 0.40, galactose 0.27, glucosamine 0.24-0.40, glucose 0.28, glucuronic acid lactone 0.20, inositol 0.24, mannitol. 0.30, quinic acid 0.42, raffinose 0.25, rhamnose 0.77, salicin 0.77, shikimic acid 0.27, sorbitol 0.29, sorbose 0.25, sucrose 0.42, xylose 0.23. Glycosides and aglycones chromatographed on buffer-impregnated paper in solvent B showed the following Rf values (ultraviolet light): quercetrin (II) 0.44, phlorizin 0.79, rutin (III) 0.29, d-catechol 0.45, fisetin 0.40, formononetin 0.91, genistein 0.86, khellin 0.92, morin 0.10, myricetin 0.15, quercetin (IV) 0.38, robinetin 0.12, tricin 0.50, dinitrophenylethanolamine 0.90, dinitrophenylglycine 0.70; II, III, and IV showed Rf 0.69, 0.29, and 0.25, resp., with BuOH-EtOH-Consden's borate buffer (Consden and Stanier C.A. 47, 664h). Many of these compds. were subjected to chromatographic techniques following horizontal paper electrophoresis, and the ratio of migration of substance to migration of dinitrophenylglycine is tabulated.

IT **138-52-3**, Salicin
(paper chromatography and electrophoresis of)

RN 138-52-3 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1953:26451 CAPLUS

DOCUMENT NUMBER: 47:26451

ORIGINAL REFERENCE NO.: 47:4513c-f

TITLE: Antiseptics for foods. LIII

AUTHOR(S): Fujikawa, Fukujiro; Sawaguchi, Gen; Takimura, Myoko

CORPORATE SOURCE: Kyoto Coll. Pharmacy

SOURCE: Yakugaku Zasshi (1952), 72, 1033-6
CODEN: YKKZAJ; ISSN: 0031-6903

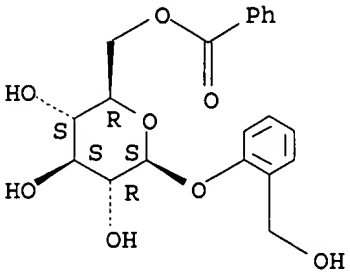
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C.A. 46, 9792h. Antiseptics for soy sauce were tested by using p-HOC6H4CO2Pr (I) as a control. Those tested were orexine (3,4-dihydro-3-phenylquinazoline) (II), II citrate, p-O2NC6H4CO2H, p-H2NC6H4CO2H, p-H2NO2SC6H4CO2H, o-(p-O2NC6H4CH:CHCO2)C6H4NO2, tibione, furacin, vitamin B1-HCl, vitamin B6-HCl, vitamin K3 (III), caperatic acid, 5,4,1,3-Me(C6H11)C6H2(OH)2 (IV), 6,4,5,1,3-Cl(C6H11)-MeC6H(OH)2 (V), 2,4,3,5-(HO)2Cl2C6HCOC4H9 (VI) and 6,2-(Me2(Et)C)C10H6OH (VIA), in which 0.005% III and 0.001% of IV, V, VIA, and VI prevented the mold growth in 60-day test, while I was effective only 5 days at 0.005% or 6 days at 0.007%. Another group of antiseptics, I, Et 6-methoxy-2-methylbenzoquinone-3-carboxylate, 2,4-HO-(H2N)C6H3CO2H, 4,1-H2NC10H6SO3Na, 2-C10H7OH, 2,4-(HO)2C6H3Ac, 2,4-(HO)2C6H3CO(CH2)3Me (VII), 2,6,4,1,3-Br2(iso-Am)C6H(ONa)2, 4,1,3(Me2EtC)C6H3(ONa)2 (VIII), bergenin, rutin, salicin, and taurine were tested, in which 0.007% VII or 0.005% VIII prevented the mold growth for 60 days, while 0.01% I was effective only for 5.5 days.

IT **99-17-2**, Salicin, 6'-benzoate
(as fungicide in soy sauce)
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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d his

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     FILE 'REGISTRY' ENTERED AT 12:17:48 ON 05 JUN 2003
L1                STRUCTURE UPLOADED
L2              2 S L1 SSS SAM
L3             96 S L1 SSS FULL

     FILE 'CAPLUS, CHEMCATS, USPATFULL' ENTERED AT 12:19:57 ON 05 JUN 2003
L4            861 S L3
L5              1 S L4 AND SALICYL ALCOHOL DERIVATIVES
L6            848 DUP REM L4 (13 DUPLICATES REMOVED)
L7              2 S L6 AND ?HYDROXYBENZOYL?
L8              0 S L6 AND ?TRIHYDROXYBENZOYL?
L9              0 S L6 AND ?TRIHYDROXYBENZOYL
L10             0 S L6 AND PHENYLPROPIONYL
L11             0 S L6 AND PHENYLPROPIONYL?
L12            11 S L6 AND PHENYLPROP?
L13            27 S L6 AND ?HYDROXYPHENYL?
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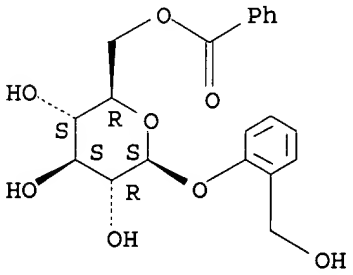
L13 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:29217 CAPLUS
DOCUMENT NUMBER: 64:29217
ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b
TITLE: Leaves of the family Salicaceae. V. The occurrence of glucosides in the leaves of Populus grandidentata
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Tappi (1965), 48(10), 607-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of P. grandidentata, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H2O and the granular ppt. filtered off. Extn. of the filtrate with Et2O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl3 and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H2O, the ppt. decompd. with H2S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H2O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H2O and 7 ml. concd. H2SO4 in 100 ml. H2O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin benzoate (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H2O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et2O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

IT **99-17-2**, Populin **138-52-3**, Salicin **529-66-8**, Tremuloidin
(in poplar leaves)

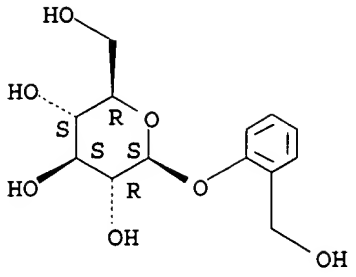
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



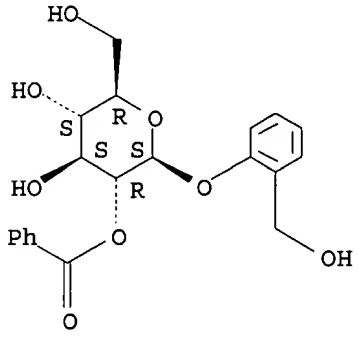
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



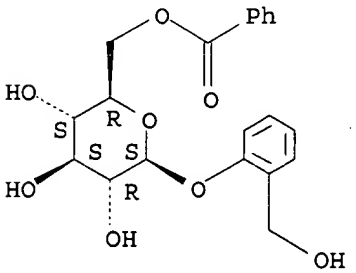
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **99-17-2**, Populin
(salicylate, in popular leaves)
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



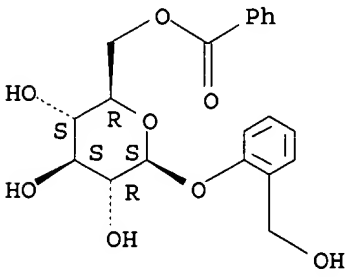
L13 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:29217 CAPLUS
DOCUMENT NUMBER: 64:29217
ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b
TITLE: Leaves of the family Salicaceae. V. The occurrence of glucosides in the leaves of Populus grandidentata
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Tappi (1965), 48(10), 607-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of P. grandidentata, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H2O and the granular ppt. filtered off. Extn. of the filtrate with Et2O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl3 and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H2O, the ppt. decompd. with H2S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H2O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H2O and 7 ml. concd. H2SO4 in 100 ml. H2O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin benzoate (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H2O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et2O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

IT **99-17-2**, Populin **138-52-3**, Salicin **529-66-8**, Tremuloidin
(in poplar leaves)

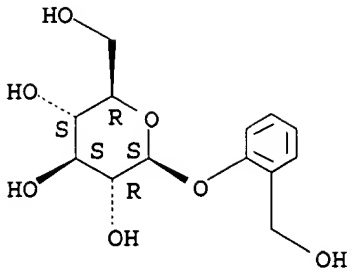
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



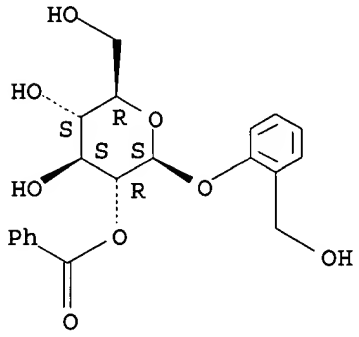
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



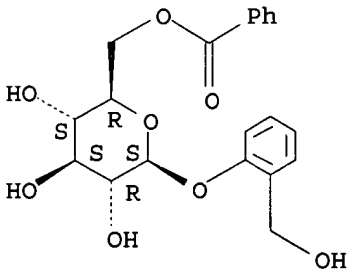
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



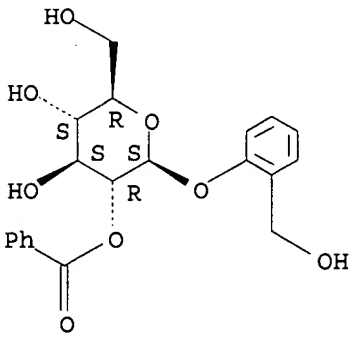
IT **99-17-2**, Populin
(salicylate, in popular leaves)
RN 99-17-2 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 6-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:634360 CAPLUS
DOCUMENT NUMBER: 117:234360
TITLE: Hemisynthesis of the naturally occurring tremuloidin
AUTHOR(S): Picard, Sophie; Bouyssou, Pascal; Chenault, Jacques
CORPORATE SOURCE: Lab. Chim. Bioorg. Anal. Assoc., Univ. Orleans, Orleans, F 45067, Fr.
SOURCE: Phytochemistry (1992), 31(8), 2909-10
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:234360
AB The hemisynthesis of tremuloidin under mild conditions by 2'-O-benzoylation of salicin is described. It appears as an essential step in synthesis of natural phenolic glycosides.
IT **529-66-8P**, Tremuloidin
RL: SPN (Synthetic preparation); PREP (Preparation)
(**prepn**. of, from salicin)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

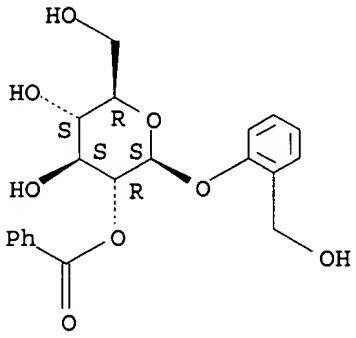
Absolute stereochemistry.



L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:403512 CAPLUS
DOCUMENT NUMBER: 111:3512
TITLE: The effect of the sample **preparation** method of extractable phenolics of Salicaceae species
AUTHOR(S): Julkunen-Tiitto, R.; Tahvanainen, J.
CORPORATE SOURCE: Dep. Biol., Univ. Joensuu, Joensuu, SF-80101, Finland
SOURCE: Planta Medica (1989), 55(1), 55-8
CODEN: PLMEAA; ISSN: 0032-0943
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effect of different tissue prehandling methods on the phenolic content of willow bark, leaves, and twigs was studied. The phenolics were extd. at room temp., purified, and analyzed by high-resoln. capillary gas chromatog. Neither oven drying at a low temp. nor room drying of fresh leaves and oven drying of bark produced any qual. changes in the glucoside compn. and only a minor binding effect was seen on the amts. of each glucoside. On the other hand, oven drying of the intact long twigs and room drying of the bark are prehandling methods to avoid. Freeze drying or immediate anal. of frozen leaves lowered the total amt. of glucosides and caused considerable qual. changes to the glucoside compn. Acetone (80%) was a slightly more effective and gentle extn. solvent for all glucosides compared with methanol.
IT **529-66-8**, Tremuloidin

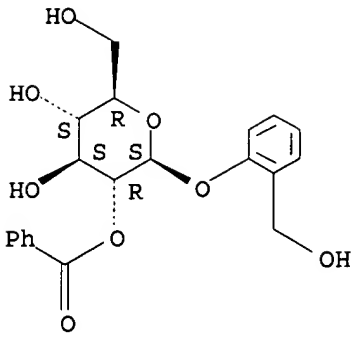
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in willow by gas chromatog., sample **prepn**. method effect on)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:489072 CAPLUS
DOCUMENT NUMBER: 109:89072
TITLE: Comparative high-performance liquid and gas-liquid chromatographic determination of phenolic glucosides in Salicaceae species
AUTHOR(S): Meier, B.; Julkunen-Tiitto, R.; Tahvanainen, J.; Sticher, O.
CORPORATE SOURCE: Dep. Pharm., Eidg. Tech. Hochsch., Zurich, CH-8092, Switz.
SOURCE: Journal of Chromatography (1988), 442, 175-86
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The phenolic glucosides of 7 willow species with different glucoside patterns were extd., purified, and analyzed by GC and HPLC. Two sample **prepn**. methods were used. It was shown that the HPLC and GC methods give comparable qual. and quant. results for the phenolic glucoside contents of the tested willows. Consequently, both methods can be used for species-specific screening of the glucoside patterns of Salicaceae species.
IT **529-66-8**, Tremuloidin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in willow species by GC and HPLC)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



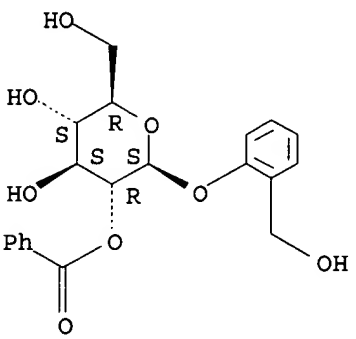
L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:514360 CAPLUS
DOCUMENT NUMBER: 67:114360
TITLE: Barks of the family Salicacaceae. XIV. Further studies on the bark of triploid Populus tremuloides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Tappi (1967), 50(7), 324-9
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. preceding abstr. The hot H2O ext. of the ground bark of P. tremuloides was concd. and extd. with EtOAc to give 5 fractions, I-V. Chromatog. over polyamide (P.C.) of I gave 1-O-p-coumaroyl-.beta.-glucose (VI), m. 205-6.degree., tremuloidin, m. 210-12.degree., and salireposide (VII), m. 198-200.degree.. Acid hydrolysis of the last eluate gave salicyloylsalicin-2 benzoate, m. 190-1.degree.. P.C. of II and III yielded VI and VII. P.C. of IV and V gave salicin. VI, [.alpha.]20D -2.5.degree. (c 3.3, 80% Me2CO) gave a pentaacetate, m. 164-5.degree. (95% EtOH), [.alpha.]20D -22.degree. (c 4, CHCl3), -23.4.degree. (c 3.3, EtOAc). Hydrolysis of VI with Ba(OH)2 on a steam bath gave p-coumaric acid (VIII). Acid hydrolysis of VI with N HCl gave VIII and glucose. Many other phenolic compds. were detected in the P.C. eluates by thin-layer chromatog. but they were not obtained in crystd. form. 28 references.

IT **529-66-8**
RL: BIOL (Biological study)
(from Populus tremuloides bark)

RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

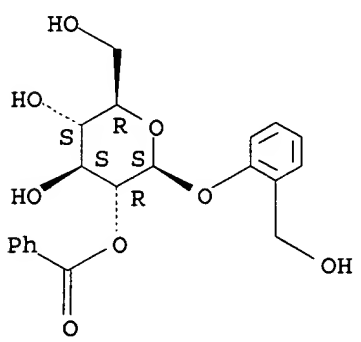


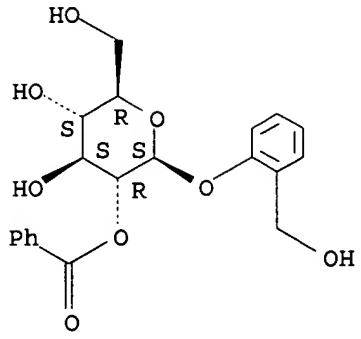
L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:488328 CAPLUS
DOCUMENT NUMBER: 67:88328
TITLE: Leaves of the family Salicaceae. IX. Components of the lead subacetate-insoluble fraction of Populus tremuloides leaves
AUTHOR(S): Kinsley, Homan, Jr.; Pearl, Irwin A.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Tappi (1967), 50(8), 419-23
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. CA 67: 54398n. Fresh P. tremuloides leaves (3070 g.), collected June 1963, were extd. with EtOH at 20.degree., and the ext. was concd. to give 793 g. conc. with 25.8% solids. The residue of 500 g. conc. in 2 l. H2O was filtered through Celite, the filtrate treated with a slurry of 100 g. Pb subacetate, the washed ppt. decompd. with H2S, and the filtrate concd. to .apprx.1 l. The soln. was washed with petroleum ether, CCl4, and C6H6 and then extd. with EtOAc. The washings were discarded. The aq. soln. contained 79% of the total solids. Polyamide chromatog. (P.C.) gave 0.01% (all based on the leaves) tremuloidin, m. 210-12.degree., 0.003% populin, m. 180-1.degree., and 0.008% salireposide, m. 203-4.degree.. P.C. of the aq. soln. gave 0.075% myo-inositol, m. 219.degree.. A similar EtOAc ext. from 2990 g. of fresh P. tremuloides leaves, collected in June 1965, contg. 18% solids, was subjected to P.C. and gave 0.003% succinic acid, 0.021% pyrocatechol, and a mixt. of flavonoid glycosides. A sample of solids was hydrolyzed with N NaOH; paper chromatog., of the hydrolyzate indicated the presence of ferulic, p-coumaric, p-hydroxybenzoic, and vanillic acids, and salicylic acid. Acid hydrolysis of the solids and paper chromatog. showed the presence of glucose, galactose, mannose, arabinose, xylose, and uronic acid. P.C. of the aq. raffinate gave 0.8% pectin, 0.012% rutin, m. 196.degree., 0.005% of an unidentified flavonoid, yellow-gray crystals, m. 239-40.degree., and 0.022% rhamnetin, yellow powder, darkening at 259.degree., m. 295.degree.. Hydrolysis of the pectin with 72% H2SO4 followed by chromatog. gave galactose, glucose, mannose, arabinose, glucuronic acid, and galacturonic acid. Acid hydrolysis of the unidentified flavonoid gave no sugars. Cellulose chromatog. of the aq. raffinate gave 0.1% of a mixt., m. 220-1.degree., of quercetin 3-glucoside and quercetin 3-galactoside. Hydrolysis of the aq. raffinate with N NaOH indicated the presence of acids, phenols, and some tar; acid hydrolysis of the aq. raffinate indicated the presence of glucose, galactose, and uronic acid. The nature of the unidentified part of the Pb-insol. materials is discussed. 25 references.

IT **529-66-8**
RL: BIOL (Biological study)
(in Populus tremuloides leaves)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

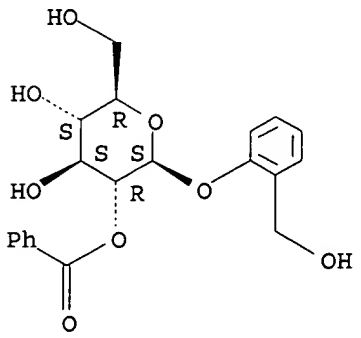
Absolute stereochemistry.





L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:454398 CAPLUS
DOCUMENT NUMBER: 67:54398
TITLE: Leaves of the family Salicaceae. VIII. Leaves of triploid Populus tremuloides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Tappi (1967), 50(4), 193-5
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 65: 9006c. Aq. extn. of 900 g. fresh leaves of P. tremuloides gave 0.1 g pyrocatechol, m. 104-5.degree., 0.254 g. tremuloidin, m. 210-11.degree., 0.67 g. a monoacetate of salicin 2-benzoate called triploside (I), m. 173-4.degree., [.alpha.]20D -1.degree. (c 3, 80% Me2CO), Rf 0.82 (20:2.2 C6H6-MeOH), and 0.1 g. salireposide, m. 145.degree. and 198-200.degree.. Acetylation of I with Ac2O-C5H5N gave a tetraacetate, m. 112-14.degree., [.alpha.]20D 34.8.degree. (c 3, CHCl3), identical with tremuloidin tetraacetate.
IT **529-66-8P**
RL: PREP (Preparation)
(from Populus tremuloides leaves)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:29217 CAPLUS
DOCUMENT NUMBER: 64:29217
ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b
TITLE: Leaves of the family Salicaceae. V. The occurrence of glucosides in the leaves of Populus grandidentata

AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Tappi (1965), 48(10), 607-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

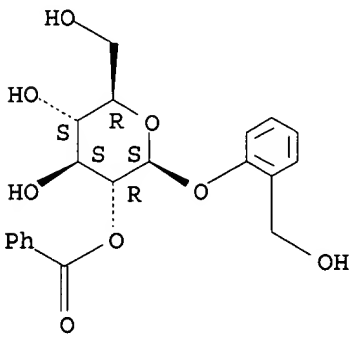
AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of P. grandidentata, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H2O and the granular ppt. filtered off. Extn. of the filtrate with Et2O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl3 and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H2O, the ppt. decompd. with H2S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H2O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H2O and 7 ml. concd. H2SO4 in 100 ml. H2O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin benzoate (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H2O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et2O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

IT **529-66-8**, Tremuloidin
(in poplar leaves)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1960:1895 CAPLUS
DOCUMENT NUMBER: 54:1895
ORIGINAL REFERENCE NO.: 54:360c-i,361a-d
TITLE: Studies on the barks of the family Salicaceae. I. Tremuloidin, a new glucoside from the bark of Populus tremuloides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Journal of Organic Chemistry (1959), 24, 731-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB A new glucoside was isolated from the bark of P. tremuloides. This glucoside, which was named tremuloidin (I), is a monobenzoate of salicin (Ia) and an isomer of populin (Ib). I was completely methylated to

tetramethyltremuloidin (II) which, in turn, was debenzoylated to a tetramethylsalicin (III) which yielded 3,4,6-tri-O-methyl-D-glucopyranoside (IV) on acid hydrolysis. Thus, I was identified as 2-benzoylsalicin. I was oxidized with dil. HNO3 to 2-benzoylhelicin (V). All products and intermediates were characterized by means of infrared absorption spectra. Fresh bark of P. tremuloides (15 kg. oven dried basis) was covered with 95% alc., left 1 week at room temp., decanted, bark treated a no. of times with alc., the combined alc. exts. filtered, concd. to 8395 g. contg. 2240 g. solids. After a few days a sample contg. 291 g. solids evapd. below 25.degree., the residue stirred with 3 l. H2O at 25.degree., left overnight, ext. decanted, and filtered through Celite, the soln. treated with excess basic Pb(OAc)2, the ppt. filtered off, the filtrate satd. with H2S, the filtrate concd. to 1500 ml., cooled, and the crystals sepd. gave 7 g. crude I. Stepwise concn. of the filtrate gave crude Ia. The yield in 3 batches was 12 g. Recrystn. of crude I gave needles, m. 207-8.degree. (H2O), [.alpha.]25D 17.1.degree. (c 3.1, C5H5N), [.alpha.]25D -12.30.degree. (c 1.5, Me2CO); tetraacetate, m. 114-150 (alc.), [.alpha.]24D 33.9.degree. (c 2.5, CHCl3). I (1 g.) left overnight at 25.degree. with 150 ml. 1% NaOH, soln. neutralized, concd. to half vol., the product filtered, washed, and recrystd. gave BzOH. The aq. filtrate afforded Ia. Ia was benzoylated and the product recrystd. to give Ib, m. 178-9.degree. (alc.), [.alpha.]24D -2.0.degree. (c 5, C5H5N), [.alpha.]25D -29.7.degree. (c 5, 80% Me2CO). Fresh leaves from P. alba extd. with hot H2O, ext. purified by basic lead acetate, H2S passed in, the filtrate evapd., and the crystals collected gave Ib, m. 179-80.degree. (H2O). Natural Ib was also isolated from the fresh bark of P. tremula. I (50 mg.) in 40 ml. 50% alc. treated with 25 to 50 ml. 0.01M Na metaperiodate, dild. to 100 ml., kept at 4.degree., aliquots taken at appropriate times for analysis. Each 5-ml. sample treated with 10 ml. satd. NaHCO3, 5 ml. 0.01M Na arsenite, and 1 ml. 1% KI, after 15 min. the remaining arsenite titrated with iodine. Data for I indicated 1 mole periodate consumed per mole I. The acidity developed detd. by a modification of the method of Abdel-Akher and Smith (C.A. 46, 11041c) in which the aliquot left 1 hr. after addn. of 10% (CH2OH)2. There was no developed acidity with I. Similar oxidn. of Ia in H2O at 25.degree. consumed 2 moles of oxidant and developed 1 mole of acid as expected. Oxidns. of Ib showed overoxidn. at 25.degree.; at 4.degree., Ib was insol. in H2O or in dil. alc. I (1 g.), 10 ml. MeI, and 15 ml. MeOH was refluxed 3 hrs. with addn. of 6 g. Ag2O, 5 ml. Me2CO added after the 2nd addn., mixt. kept overnight at room temp., the filtrate evapd., the sirup dissolved in 10 ml. MeI and a few drops of MeOH and methylated as before. The process repeated 3 times gave 1.05 g. II, viscous oil, [.alpha.]25D 6.56.degree. (c 4.2, CHCl3). All attempts to crystallize II failed. Upon hydrolysis with HCl, paper-chromatography of the hydrolyzate showed only a trimethylglucose. II (1.05 g.) in 20 ml. MeOH refluxed 10 min. with 0.1 g. Na in 10 ml. MeOH, dild. with 30 ml. H2O, and partially evapd. gave 0.31 g. .omega.,3,4,6-tetramethylsalicin (III), m. 85-6.degree., [.alpha.]25D -39.1.degree. (c 1.2, CHCl3). The aq. layer acidified and left at room conditions gave BzOH. III (0.35 g.), 4 ml. MeOH, and 6 ml. 2N HCl refluxed 2 hrs., MeOH removed, the residue filtered, the filtrate treated with excess IR-4B ion exchange resin, the combined filtrate and washings evapd. gave a sirup. Paper-chromatography indicated only a trimethylglucose and some phenolic aglucon material with good sepn. The entire sirup in 2.5 ml. MeOH was streaked on four 8-in. wide papers, previously washed with MeOH, the papers were developed in EtOAc-AcOH-H2O, the located bands cut out, these bands eluted with MeOH, and the eluate evapd. to yield a sirup which crystd. to IV, m. 97-8.degree. (iso-Pr2O). The Ag spray procedure indicated the glucosides under study as dark brown spots. In the present modification the paper after standing at room temp. was bathed a few times in concd. Na2S2O3 soln., washed with H2O, and dried. The glucosides appeared as black spots. The 3 glucosides Ia, Ib, and I were easily recognized. Rf values for EtOAc-AcOH-H2O were: Ia, 0.60; Ib, 0.84, I, 0.85. The residue remaining after extn. at 25.degree. as noted above of P. tremuloides covered with 1 l. hot H2O, mixt. refluxed

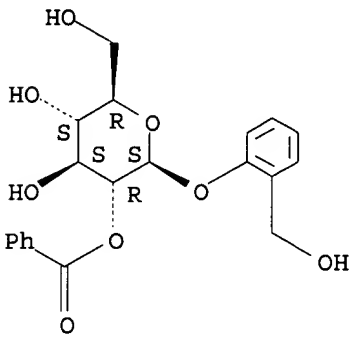
1 hr., cooled, decanted, the extn. repeated on the heavy oil, the combined aq. exts. filtered, purified by means of basic lead acetate, then with H2S, the soln. concd., and cooled gave 2.8 g. I. The filtrate gave 0.8 g. of a mixt. of 75% I and 25% Ib. Another concn. gave 4.1 g. 50% mixt. of I and Ib. A mixt. of I and Ib (0.1 g.) in the above developer chromatographed on paper gave pure I, I with a trace of Ib, pure Ib, and impure Ib. The infrared absorption spectra were given for the above compds. in KBr pellets.

IT **529-66-8**, Tremuloidin
(isolation from bark of Populus tremuloides, and tetraacetate)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FILE 'REGISTRY' ENTERED AT 18:10:44 ON 05 JUN 2003
L1 1 S 529-66-8

FILE 'CAPLUS, USPATFULL, CA, CAOLD' ENTERED AT 18:11:45 ON 05 JUN 2003
L2 100 S L1
L3 55 DUP REM L2 (45 DUPLICATES REMOVED)
L4 8 S L3 AND PREPARATION

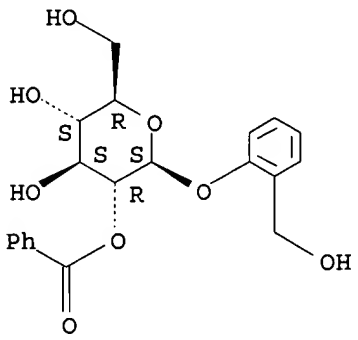
L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:634360 CAPLUS
DOCUMENT NUMBER: 117:234360
TITLE: Hemisynthesis of the naturally occurring tremuloidin
AUTHOR(S): Picard, Sophie; Bouyssou, Pascal; Chenault, Jacques
CORPORATE SOURCE: Lab. Chim. Bioorg. Anal. Assoc., Univ. Orleans, Orleans, F 45067, Fr.
SOURCE: Phytochemistry (1992), 31(8), 2909-10
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:234360

AB The hemisynthesis of tremuloidin under mild conditions by 2'-O-benzoylation of salicin is described. It appears as an essential step in **synthesis** of natural phenolic glycosides.

IT **529-66-8P**, Tremuloidin
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, from salicin)

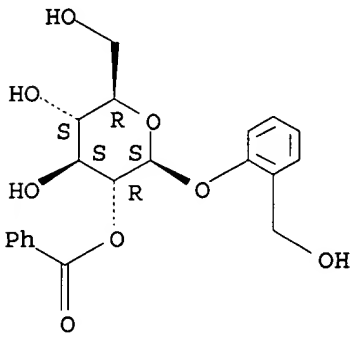
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



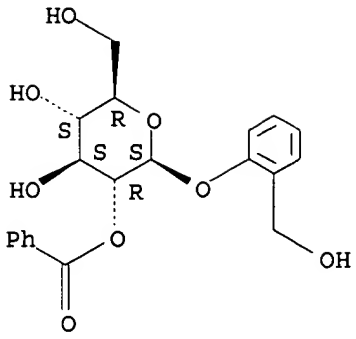
L6 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:493550 CAPLUS
DOCUMENT NUMBER: 107:93550
TITLE: Chemical constituents of Chinese white poplar (Populus tomentosa) leaf
AUTHOR(S): Ma, Tianbo; Li, Mengguang; Li, Junlin; Liu, Shanxin; Wang, Aiqin
CORPORATE SOURCE: Shandong Coll. Tradit. Chin. Med., Jinan, Peop. Rep. China
SOURCE: Zhongcaoyao (1987), 18(3), 105-7
CODEN: CTYAD8; ISSN: 0253-2670
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT **529-66-8**, Tremuloidin
RL: BIOL (Biological study)
(from Populus tomentosa)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



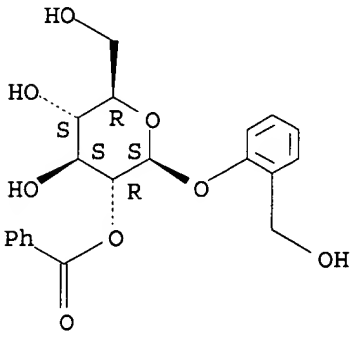
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1962:26757 CAPLUS
DOCUMENT NUMBER: 56:26757
ORIGINAL REFERENCE NO.: 56:5126b-e
TITLE: The barks of the family Salicaceae. IV. Preliminary evaluation for glucosides of barks of several species of the genus Populus
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.; DeHaas, Herman; Loving, Ben A.; Scott, Donald A.; Turley, Roy H.; Werth, Richard E.
CORPORATE SOURCE: Inst. Paper Chem., Appleton, WI
SOURCE: Tappi (1961), 44, 475-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **529-66-8**, Tremuloidin
(from poplar bark)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1960:122069 CAPLUS
DOCUMENT NUMBER: 54:122069
ORIGINAL REFERENCE NO.: 54:23318f-h
TITLE: The methanol-extractable aromatic materials in the inner bark of Populus tremuloides
AUTHOR(S): Faber, Horace B., Jr.
CORPORATE SOURCE: Inst. Paper Chem., Appleton, WI
SOURCE: Tappi (1960), 43, 406-13
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT **529-66-8**, Tremuloidin
(detection in aspen inner bark)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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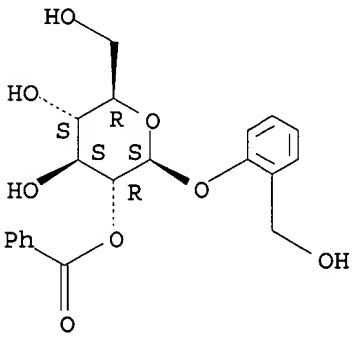
FILE 'REGISTRY' ENTERED AT 18:10:44 ON 05 JUN 2003
L1 1 S 529-66-8

FILE 'CAPLUS, USPATFULL, CA, CAOLD' ENTERED AT 18:11:45 ON 05 JUN 2003
L2 100 S L1
L3 55 DUP REM L2 (45 DUPLICATES REMOVED)
L4 8 S L3 AND PREPARATION
L5 1 S L3 AND SYNTHESIS
L6 3 S L3 AND BENZOIC ACID

L7 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:493550 CAPLUS
DOCUMENT NUMBER: 107:93550
TITLE: Chemical constituents of Chinese white poplar (Populus tomentosa) leaf
AUTHOR(S): Ma, Tianbo; Li, Mengguang; Li, Junlin; Liu, Shanxin; Wang, Aiqin
CORPORATE SOURCE: Shandong Coll. Tradit. Chin. Med., Jinan, Peop. Rep. China
SOURCE: Zhongcaoyao (1987), 18(3), 105-7
CODEN: CTYAD8; ISSN: 0253-2670
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Populin, tremuloidin, salicin, and benzoic acid were identified from the leaves of P. tomentosa. NMR, IR, and mass spectrometry were used for the identification.
IT **529-66-8**, Tremuloidin
RL: BIOL (Biological study)
(from Populus tomentosa)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

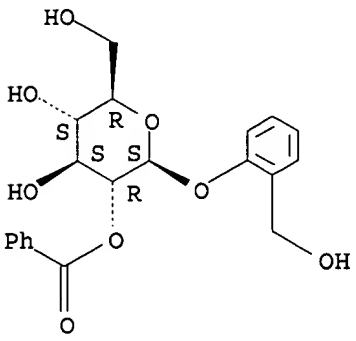
Absolute stereochemistry.



L7 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1972:549716 CAPLUS
DOCUMENT NUMBER: 77:149716
TITLE: Phytochemistry of the Salicaceae. IV. Bark of Salix petiolaris (S. gracilis var textoris)
AUTHOR(S): Steele, J. W.; Weitzel, P. F.; Audette, R. C. S.
CORPORATE SOURCE: Fac. Pharm., Univ. Manitoba, Winnipeg, MB, Can.
SOURCE: Journal of Chromatography (1972), 71(3), 435-41
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB November bark of S. petiolaris Sm. was extd. with Me2CO and EtOH and the exts. were subjected to chromatog. on polyamide columns. The various column fractions were monitored by thin-layer and gas-liq. chromatog. procedures. From these results and by isolation of cryst. material, the bark was shown to contain salicin, picein, vimalin, salicyloylsalicin, salireposide, grandidentatin, populin, tremulacin and (or) tremuloidin, salicyloylsalicin-2-O-**benzoate**, (+)-catechin, and .beta.-sitosterol.
IT **529-66-8**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of willow bark)

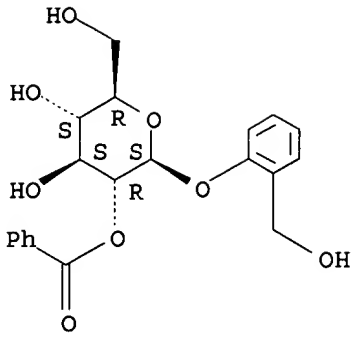
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



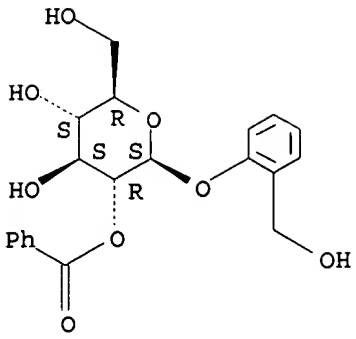
L7 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:514360 CAPLUS
DOCUMENT NUMBER: 67:114360
TITLE: Barks of the family Salicacaceae. XIV. Further studies on the bark of triploid Populus tremuloides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Tappi (1967), 50(7), 324-9
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. preceding abstr. The hot H2O ext. of the ground bark of P. tremuloides was concd. and extd. with EtOAc to give 5 fractions, I-V. Chromatog. over polyamide (P.C.) of I gave 1-O-p-coumaroyl-.beta.-glucose (VI), m. 205-6.degree., tremuloidin, m. 210-12.degree., and salireposide (VII), m. 198-200.degree.. Acid hydrolysis of the last eluate gave salicyloylsalicin-2 **benzoate**, m. 190-1.degree.. P.C. of II and III yielded VI and VII. P.C. of IV and V gave salicin. VI, [.alpha.]20D -2.5.degree. (c 3.3, 80% Me2CO) gave a pentaacetate, m. 164-5.degree. (95% EtOH), [.alpha.]20D -22.degree. (c 4, CHCl3), -23.4.degree. (c 3.3, EtOAc). Hydrolysis of VI with Ba(OH)2 on a steam bath gave p-coumaric acid (VIII). Acid hydrolysis of VI with N HCl gave VIII and glucose. Many other phenolic compds. were detected in the P.C. eluates by thin-layer chromatog. but they were not obtained in crystd. form. 28 references.
IT **529-66-8**
RL: BIOL (Biological study)
(from Populus tremuloides bark)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



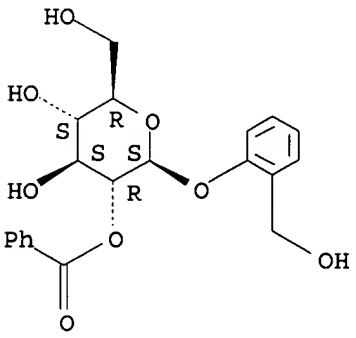
L7 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:514359 CAPLUS
DOCUMENT NUMBER: 67:114359
TITLE: Barks of the family Salicaceae. XIII. Hot-water extractives of the green bark of Populus trichocarpa
AUTHOR(S): Estes, Timothy K.; Pearl, Irwin A.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Tappi (1967), 50(7), 318-24
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 65: 9006c. The oven-dry ground bark of P. trichocarpa (1.5 kg.) was extd. with 20 l. hot H2O, the ext. filtered over Celite, and concd. in vacuo to .apprx.2 l. contg. 16% of the bark. The ext. was exhaustively extd. with CHCl3, Et2O, and EtOAc, giving the extractives I (8%), II (10%), and III (20%), resp. The final raffinate (IV) contained 62% of the hot H2O extractives. I was triturated with EtOH and the waxy residue discarded. I was then sepd. with Pb subacetate into 17% of a "Pb-sol." fraction, Ia, and 49% of a "Pb-insol." fraction, Ib. By polyamide chromatog. (P.C.) of Ia, salicin (V), salicyl alc. (VI), and tremuloidin (VII) and a mixt. of trichocarpin (VIII) and salireposide (IX) were isolated. P.C. of Ib indicated the presence of pyrocatechol, V, VI, VIII, and IX. Acid hydrolysis of I gave no salicyloylsalicin deriv. P.C. of II gave VIII, IX, p-coumaric acid (X), and trichocarposide (XI), m. 180-2.degree. (H2O), [.alpha.]20D -11.4.degree. (c 2.3, 80% Me2CO). Pb subacetate treatment of II gave VIII, IX, X, and XI. Pb subacetate and P.C. of II gave VIII, IX, X, and XI. Mild hydrolysis and P.C. of III indicated the presence of salicyloylsalicin-2 **benzoate** and X. P.C. of IV indicated the presence of glucose, fructose, and sucrose. Alk. hydrolysis of XI gave III and X; periodate oxidn. of XI consumed 2 moles with the liberation of 1 mole HCO2H. Hydrolysis of XI with .beta.-glucosidase gave no glucose. 21 references.
IT **529-66-8**
RL: BIOL (Biological study)
(from Populus trichocarpa bark)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:454398 CAPLUS
DOCUMENT NUMBER: 67:54398
TITLE: Leaves of the family Salicaceae. VIII. Leaves of triploid Populus tremuloides
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI, USA
SOURCE: Tappi (1967), 50(4), 193-5
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 65: 9006c. Aq. extn. of 900 g. fresh leaves of P. tremuloides gave 0.1 g pyrocatechol, m. 104-5.degree., 0.254 g. tremuloidin, m. 210-11.degree., 0.67 g. a monoacetate of salicin 2-**benzoate** called triploside (I), m. 173-4.degree., [.alpha.]20D -1.degree. (c 3, 80% Me2CO), Rf 0.82 (20:2.2 C6H6-MeOH), and 0.1 g. salireposide, m. 145.degree. and 198-200.degree.. Acetylation of I with Ac2O-C5H5N gave a tetraacetate, m. 112-14.degree., [.alpha.]20D 34.8.degree. (c 3, CHCl3), identical with tremuloidin tetraacetate.
IT **529-66-8P**
RL: PREP (Preparation)
(from Populus tremuloides leaves)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L7 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:447991 CAPLUS
DOCUMENT NUMBER: 65:47991

ORIGINAL REFERENCE NO.: 65:9006c-g
TITLE: Barks of the family Salicaceae. XII. Leaves of the family Salicaceae. 7. Glucosides from the barks and leaves of triploid varieties of Populus species
AUTHOR(S): Pearl, I. A.; Darling, S. F.; Heller, S. F.
CORPORATE SOURCE: Lignin Chem. Group, Inst. of Paper Chemistry, Appleton, WI
SOURCE: Tappi (1966), 49(6), 278-80
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

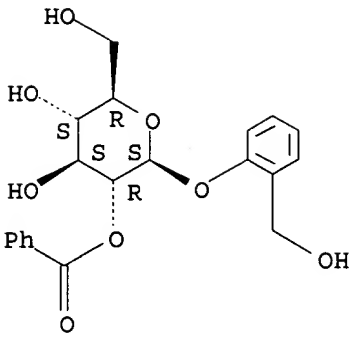
AB cf. CA 64, 797b; 65, 1042d. Fresh leaves (4.5 kg. = 1.8 kg. dry leaves) of triploid P. tremuloides (TPT) were extd. with hot H2O, half the ext. was immediately treated with a hot soln. of 165 g. Pb subacetate (I) and the filtered and deleaded soln. concd. in vacuo to give 9 g. populin (II), m. 180-1.degree.. The other half was concd. in vacuo to 1 l. and centrifuged, the waxy ppt. dissolved in EtOH, and the filtered soln. evapd. to give 5.7 g. II, m. 182-3.degree.. The centrifuged aq. soln. was then exhaustively extd. with CHCl3 and the ext. concd. to give 4.21 g. tremuloidin (III), m. 200-5.degree.. The CHCl3 mother liquor was evapd. in vacuo to give 44 g. green viscous sirup (IV). IV (22 g.) was dissolved in 175 ml. EtOH, 1.5 l. H2O added, the soln. filtered through Celite, a hot soln. of 50 g. I added to the hot filtrate, the filtered soln. kept overnight, deleaded with H2S, filtered, and concd. in vacuo to give 1.7 g. II. From the mother liquor 0.4 g. salicin (V), m. 190-3.degree., was isolated. IV (22 g.) in 175 ml. EtOH and 1.5 l. H2O was refluxed 0.5 hr. with 32 g. concd. H2SO4, the EtOH distd. in vacuo, and the aq. soln. kept a few days to give 20 mg. mixt. of salicyloylsalicin (VI) 2-**benzoate** (VII) and VI, as shown by thin layer chromatography (TLC). The original CHCl3-extd. aq. soln. was freed of CHCl3 and exhaustively extd. with EtOAc to give 4.64 g. V, m. 195-6.degree.. Leaves (7 kg. = 2.8 kg. dry material) of diploid P. tremuloides (DPT) were extd. with hot H2O, the ext. was treated with I, and the deleaded filtrate concd. in vacuo to .apprx.1.5 l. to give 1.6 g. II. The hot H2O ext. of 2 kg. of DPT leaves was filtered through Celite, the filtrate concd. in vacuo to 1.5 l., and the centrifuged soln. allowed to stand, but no II sepd. The bark (1080 g. = 1 kg. oven-dried material) of TPT was extd. with hot H2O, the ext. concd. to 1 l. and extd. exhaustively with CHCl3 to give 64 g. olive green sirup. This was refluxed 35 min. in 500 ml. H2O and 250 ml. 95% EtOH with 32 g. concd. H2SO4 and the mixt. kept overnight to give 14.6 g. crude VII. The mother liquor was concd. in vacuo and extd. with Et2O, and the dried ext. evapd. to give 8.81 g. yellow mixt. from which some BzOH sepd. From the aq. raffinate some VI and VII sepd. as shown by TLC. The raffinate was exhaustively extd. with EtOAc and the ext. evapd. to give a yellow sirup from which 4.84 g. V was isolated. Evapn. of the mother liquor gave 150 g. EtOAc exts. This (90 g.) in 2250 ml. hot H2O was treated with 50 g. I in 250 ml. H2O, the filtered soln. was deleaded with H2S and concd. in vacuo to 250 ml. to give 5.57 g. salireposide, m. 150-4.degree., resolidifying and m. again at 200-2.degree.. From the mother liquor 14.6 g. V was isolated. Extn. of 1.08 kg. bark with hot H2O, treatment of the ext. with I, and work-up gave 7.5 g. III. Extn. of 146 g. dry leaves of TPT and concn. of the ext. gave 0.25 g. II. An identical extn. of DPT leaves gave 0.044% II. The significance of these results was discussed.

IT **529-66-8**, Tremuloidin
(from Populus tremuloides)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1966:29217 CAPLUS
DOCUMENT NUMBER: 64:29217
ORIGINAL REFERENCE NO.: 64:5449g-h,5450a-b
TITLE: Leaves of the family Salicaceae. V. The occurrence of glucosides in the leaves of Populus grandidentata
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Tappi (1965), 48(10), 607-8
CODEN: TAPPAP; ISSN: 0039-8241
DOCUMENT TYPE: Journal
LANGUAGE: English

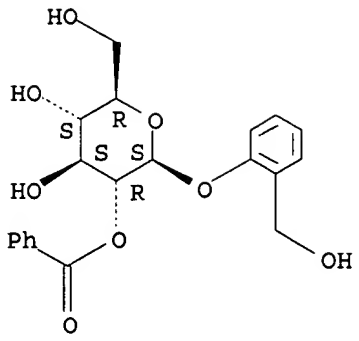
AB cf. CA 64, 797b. The EtOH ext. of 518 g. leaves of P. grandidentata, collected in June, was evapd. and yielded 133 g. sirup which was stirred with 2 l. H2O and the granular ppt. filtered off. Extn. of the filtrate with Et2O and evapn. of the ext. gave a mixt. of BzOH and pyrocatechol. The concd. aq. soln. was extd. with CHCl3 and the ext. concd., giving 2.26 g. cryst. solid (I). Exhaustive extn. of the aq. soln. with EtOAc for 10, 30, 60, and 140 hrs. gave 5 g. polyphenolic material, 0.6 and 0.95 g. oligomeric material, consisting partially of salicin (II), and 1.72 g. II, resp. The aq. soln. was then dild. to 3 l. and treated with 50 g. Pb subacetate in 100 ml. H2O, the ppt. decompd. with H2S, and the filtered soln. evapd. in vacuo to give 0.375 g. quercitin-3-glucosiduronic acid, m. 193-5.degree. (H2O). The filtrate of I was evapd. in vacuo, the residue dissolved in 50 ml. EtOH; 150 ml. H2O and 7 ml. concd. H2SO4 in 100 ml. H2O were added, and the mixt. was refluxed 0.5 hr. and concd. in vacuo, giving 0.263 g. salicyloylsalicin **benzoate** (III), m. 188-90.degree. (95% EtOH). Countercurrent distribution of I between EtOAc and H2O gave 0.85 g. tremuloidin, m. 212-13.degree. and 0.24 g. populin (IV), m. 181-3.degree.. Extn. of 471 g. dry leaves with Et2O gave 120 g. solid from which 1.1 g. III, and some IV and II were isolated.

IT **529-66-8**, Tremuloidin
(in poplar leaves)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

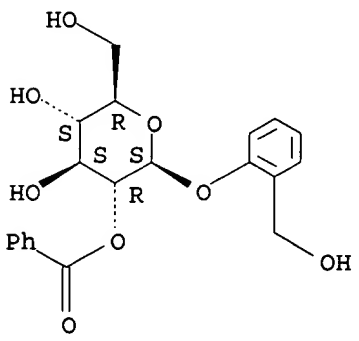


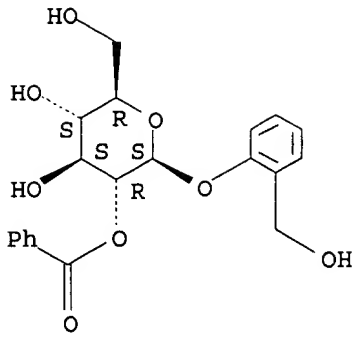
L7 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1964:447167 CAPLUS
DOCUMENT NUMBER: 61:47167
ORIGINAL REFERENCE NO.: 61:8131h,8132a-b
TITLE: The phenolic glycosides of the Salicaceae. II. Isolation and detection
AUTHOR(S): Thieme, Heinz
CORPORATE SOURCE: Karl-Marx Univ., Leipzig, Germany
SOURCE: Pharmazie (1964), 19(7), 471-5
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 60, 9098e. The phenolic glycosides (from Salix spp.: salicin, populin, tremuloidin, fragilin, picein, salireposide, grandidentatin, triandrin; from Populus: glycosmin and salicylpopulin ((salicyloyl-tremuloidin (Pearl, J. Org. Chem. 27, 1806(1962)) were obtained by fractional crystn. from leaf and bark exts. obtained by continuous percolation in perforators with AcOEt (sepn. of sugars) and polyamide column chromatography (sepn. of tannins and flavone glycosides). The glycosidal mixt. thus obtained was sepd. by cellulose column chromatography. Characterization of the individual glycosides is possible by detn. of m.ps., [.alpha.] of the compds. and their Ac derivs., infrared absorption spectra (given for the 8 Salix glycosides), and by identification of hydrolytic products formed by fermentative or alk. hydrolysis. For identification of the glycosides present in various Salix or Populus spp., a paper chromatographic method is described. BuOH-xylene-AcOH-H2O (6:4:2:8), and Millon's reagent are used, followed by drying at 95.degree.. The Rf values and differential spot colors permit ready differentiation of the 8 compds.

IT **529-66-8**, Tremuloidin
(detection and sepn. of)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



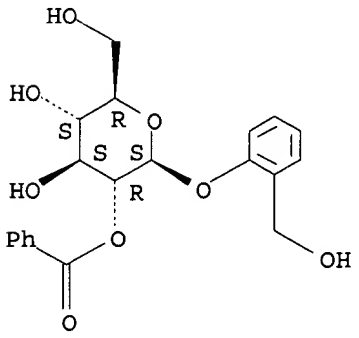


L7 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1963:470451 CAPLUS
DOCUMENT NUMBER: 59:70451
ORIGINAL REFERENCE NO.: 59:13110g-h
TITLE: Leaves of the family Salicaceae. III. Migration of acyl groups during isolation of glycosides from Populus grandidentata leaves
AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI
SOURCE: Archives of Biochemistry and Biophysics (1963), 102(1), 33-8
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 59, 2931b. It was found that mild alkali, such as Pb subacetate, causes migration of the benzoyl group from the 2 position on tremuloidin to the 6 position on populin at elevated temps. The tremuloidin was obtained from P. grandidentata. Purification of aq. exts. with Pb subacetate at elevated temps. gives populin whereas at room temp. tremuloidin is obtained. MgO also causes rearrangement of the benzoyl groups in tremuloidin and in the **benzoate** of salicyloyl salicin.

IT **529-66-8**, Tremuloidin
(from Populus grandidentata, benzoyl group migration during isolation in alkali)
RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1960:1895 CAPLUS
DOCUMENT NUMBER: 54:1895
ORIGINAL REFERENCE NO.: 54:360c-i,361a-d

TITLE: Studies on the barks of the family Salicaceae. I. Tremuloidin, a new glucoside from the bark of Populus tremuloides

AUTHOR(S): Pearl, Irwin A.; Darling, Stephen F.
CORPORATE SOURCE: Inst. of Paper Chem., Appleton, WI

SOURCE: Journal of Organic Chemistry (1959), 24, 731-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB A new glucoside was isolated from the bark of P. tremuloides. This glucoside, which was named tremuloidin (I), is a monobenzoate of salicin (Ia) and an isomer of populin (Ib). I was completely methylated to tetramethyltremuloïdin (II) which, in turn, was debenzoylated to a tetramethylsalicin (III) which yielded 3,4,6-tri-O-methyl-D-glucopyranoside (IV) on acid hydrolysis. Thus, I was identified as 2-benzoylsalicin. I was oxidized with dil. HNO3 to 2-benzoylhelicin (V). All products and intermediates were characterized by means of infrared absorption spectra. Fresh bark of P. tremuloides (15 kg. oven dried basis) was covered with 95% alc., left 1 week at room temp., decanted, bark treated a no. of times with alc., the combined alc. exts. filtered, concd. to 8395 g. contg. 2240 g. solids. After a few days a sample contg. 291 g. solids evapd. below 25.degree., the residue stirred with 3 l. H2O at 25.degree., left overnight, ext. decanted, and filtered through Celite, the soln. treated with excess basic Pb(OAc)2, the ppt. filtered off, the filtrate satd. with H2S, the filtrate concd. to 1500 ml., cooled, and the crystals sepd. gave 7 g. crude I. Stepwise concn. of the filtrate gave crude Ia. The yield in 3 batches was 12 g. Recrystn. of crude I gave needles, m. 207-8.degree. (H2O), [.alpha.]25D 17.1.degree. (c 3.1, C5H5N), [.alpha.]25D -12.30.degree. (c 1.5, Me2CO); tetraacetate, m. 114-150 (alc.), [.alpha.]24D 33.9.degree. (c 2.5, CHCl3). I (1 g.) left overnight at 25.degree. with 150 ml. 1% NaOH, soln. neutralized, concd. to half vol., the product filtered, washed, and recrystd. gave BzOH. The aq. filtrate afforded Ia. Ia was benzoylated and the product recrystd. to give Ib, m. 178-9.degree. (alc.), [.alpha.]24D -2.0.degree. (c 5, C5H5N), [.alpha.]25D -29.7.degree. (c 5, 80% Me2CO). Fresh leaves from P. alba extd. with hot H2O, ext. purified by basic lead acetate, H2S passed in, the filtrate evapd., and the crystals collected gave Ib, m. 179-80.degree. (H2O). Natural Ib was also isolated from the fresh bark of P. tremula. I (50 mg.) in 40 ml. 50% alc. treated with 25 to 50 ml. 0.01M Na metaperiodate, dild. to 100 ml., kept at 4.degree., aliquots taken at appropriate times for analysis. Each 5-ml. sample treated with 10 ml. satd. NaHCO3, 5 ml. 0.01M Na arsenite, and 1 ml. 1% KI, after 15 min. the remaining arsenite titrated with iodine. Data for I indicated 1 mole periodate consumed per mole I. The acidity developed detd. by a modification of the method of Abdel-Akher and Smith (C.A. 46, 11041c) in which the aliquot left 1 hr. after addn. of 10% (CH2OH)2. There was no developed acidity with I. Similar oxidn. of Ia in H2O at 25.degree. consumed 2 moles of oxidant and developed 1 mole of acid as expected. Oxidns. of Ib showed overoxidn. at 25.degree.; at 4.degree., Ib was insol. in H2O or in dil. alc. I (1 g.), 10 ml. MeI, and 15 ml. MeOH was refluxed 3 hrs. with addn. of 6 g. Ag2O, 5 ml. Me2CO added after the 2nd addn., mixt. kept overnight at room temp., the filtrate evapd., the sirup dissolved in 10 ml. MeI and a few drops of MeOH and methylated as before. The process repeated 3 times gave 1.05 g. II, viscous oil, [.alpha.]25D 6.56.degree. (c 4.2, CHCl3). All attempts to crystallize II failed. Upon hydrolysis with HCl, paper-chromatography of the hydrolyzate showed only a trimethylglucose. II (1.05 g.) in 20 ml. MeOH refluxed 10 min. with 0.1 g. Na in 10 ml. MeOH, dild. with 30 ml. H2O, and partially evapd. gave 0.31 g. .omega.,3,4,6-tetramethylsalicin (III), m. 85-6.degree., [.alpha.]25D -39.1.degree. (c 1.2, CHCl3). The aq. layer acidified and left at room conditions gave BzOH. III (0.35 g.), 4 ml. MeOH, and 6 ml. 2N HCl refluxed 2 hrs., MeOH removed, the residue filtered, the filtrate treated with excess IR-4B ion exchange resin, the combined filtrate and washings evapd. gave a sirup. Paper-chromatography indicated only a

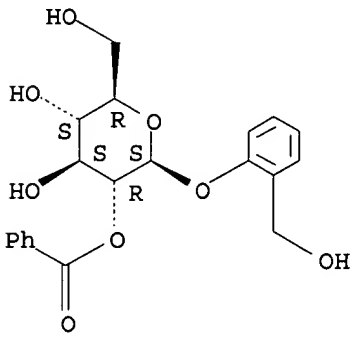
trimethylglucose and some phenolic aglucon material with good sepn. The entire sirup in 2.5 ml. MeOH was streaked on four 8-in. wide papers, previously washed with MeOH, the papers were developed in EtOAc-AcOH-H2O, the located bands cut out, these bands eluted with MeOH, and the eluate evapd. to yield a sirup which crystd. to IV, m. 97-8.degree. (iso-Pr2O). The Ag spray procedure indicated the glucosides under study as dark brown spots. In the present modification the paper after standing at room temp. was bathed a few times in concd. Na2S2O3 soln., washed with H2O, and dried. The glucosides appeared as black spots. The 3 glucosides Ia, Ib, and I were easily recognized. Rf values for EtOAc-AcOH-H2O were: Ia, 0.60; Ib, 0.84, I, 0.85. The residue remaining after extn. at 25.degree. as noted above of P. tremuloides covered with 1 l. hot H2O, mixt. refluxed 1 hr., cooled, decanted, the extn. repeated on the heavy oil, the combined aq. exts. filtered, purified by means of basic lead acetate, then with H2S, the soln. concd., and cooled gave 2.8 g. I. The filtrate gave 0.8 g. of a mixt. of 75% I and 25% Ib. Another concn. gave 4.1 g. 50% mixt. of I and Ib. A mixt. of I and Ib (0.1 g.) in the above developer chromatographed on paper gave pure I, I with a trace of Ib, pure Ib, and impure Ib. The infrared absorption spectra were given for the above compds. in KBr pellets.

IT **529-66-8**, Tremuloidin
(isolation from bark of Populus tremuloides, and tetraacetate)

RN 529-66-8 CAPLUS

CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

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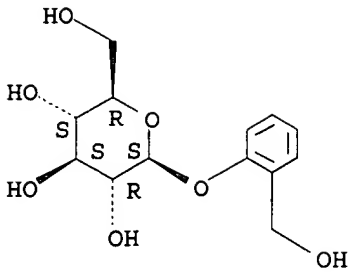
FILE 'REGISTRY' ENTERED AT 18:10:44 ON 05 JUN 2003
L1 1 S 529-66-8

FILE 'CAPLUS, USPATFULL, CA, CAOLD' ENTERED AT 18:11:45 ON 05 JUN 2003
L2 100 S L1
L3 55 DUP REM L2 (45 DUPLICATES REMOVED)
L4 8 S L3 AND PREPARATION
L5 1 S L3 AND SYNTHESIS
L6 3 S L3 AND BENZOIC ACID
L7 10 S L3 AND BENZOATE



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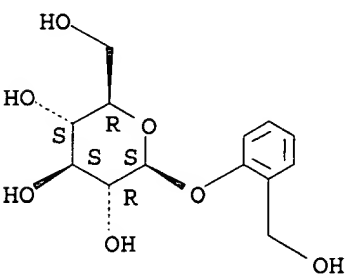
L5 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:490843 CAPLUS
DOCUMENT NUMBER: 135:223662
TITLE: Testing the effects of drying methods on willow flavonoids, tannins, and salicylates
AUTHOR(S): Julkunen-Tiitto, Riitta; Sorsa, Sinikka
CORPORATE SOURCE: Department of Biology, University of Joensuu, Joensuu, FIN-80101, Finland
SOURCE: Journal of Chemical Ecology (2001), 27(4), 779-789
CODEN: JCECD8; ISSN: 0098-0331
PUBLISHER: Kluwer Academic/Plenum Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In this study, we compared the effects of several preservation methods on the secondary phenolics of the mature leaves of purple willow (Salix purpurea L., Salicaceae) with results obtained with fresh leaf analyses. Conventional freeze-drying, in which the leaves were first frozen with liq. nitrogen and then placed in a freeze-dryer, produced substantial qual. and quant. changes in purple willow flavonoids and salicylates. Modified freeze-drying, in which leaves were put into a freeze-dryer without being prefrozen, gave concns. that, for most secondary components, were comparable with those found in fresh leaves. Reducing the freeze-dryer chamber temp. hindered the decompn. of phenolics in prefrozen leaves and in leaves dried without prefreezing. Heat drying induced substantial changes in the compn. of all phenolics, except for apigenin-7-glucoside. Vacuum drying at room temp. gave the highest concns. for nearly all phenolics, while room-drying with desiccation gave results that were comparable with those obtained by fresh leaf analyses.

IT **138-52-3**, Salicin **529-66-8**, Tremuloidin
29836-40-6, Tremulacin **29836-41-7**, Salicortin
RL: ANT (Analyte); ANST (Analytical study)
(testing the effects of drying methods on willow flavonoids, tannins, and salicylates)

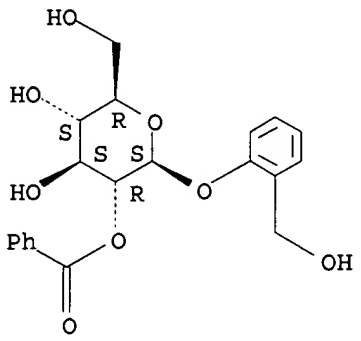
RN 138-52-3 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

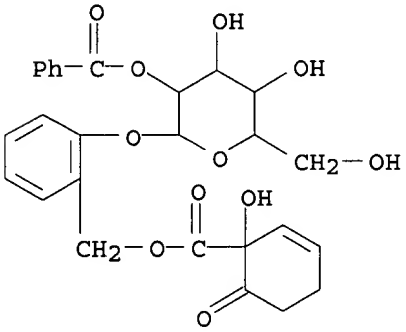


RN 529-66-8 CAPLUS
CN .beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl, 2-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

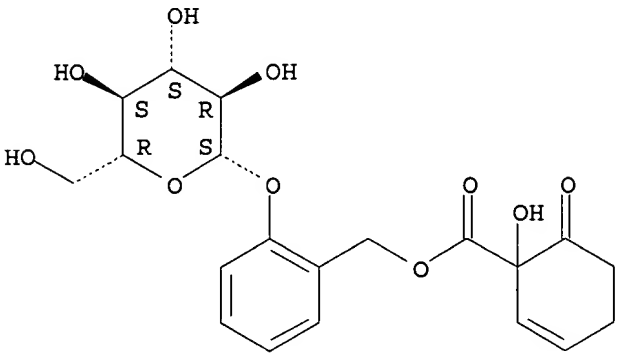


RN 29836-40-6 CAPLUS
CN .beta.-D-Glucopyranoside, 2-[[[(1-hydroxy-6-oxo-2-cyclohexen-1-yl)carbonyl]oxy]methyl]phenyl, 2-benzoate (9CI) (CA INDEX NAME)



RN 29836-41-7 CAPLUS
CN .beta.-D-Glucopyranoside, 2-[[[(1-hydroxy-6-oxo-2-cyclohexen-1-yl)carbonyl]oxy]methyl]phenyl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2002 ACS